The Error for Quadrature Methods: A Complex Variables Approach

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By a quadrature method for integration over an interval $[a, b]$, we mean a set of distinct points $x_0 < x_1 < \cdots < x_n$, a set of constants $\alpha_0, \ldots, \alpha_n$, and a formula

$$Q_n(f) := \sum_{j=0}^{n} \alpha_j f(x_j) \tag{1}$$

that serves as an estimate of the integral

$$\int_a^b f(x)\, dx.$$

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In this note, we present a new proof of a recent result [3] due to Claus Schneider that provides a simple and elegant method for determining the error and degree of precision for general quadrature formulae. The essential feature of our proof is the use of complex variable techniques, which simplify the algebraic manipulation of divided differences, and provide a straightforward derivation of a formula for the error

$$E_n(f) := \int_a^b f(x)\,dx - Q_n(f).$$

We shall prove

THEOREM 1 [3: Prop. 2.1]. *Let* $x_0 < x_1 < \cdots < x_u = a < \cdots < x_v = b < \cdots < x_n$, *and let* $Q_n(f)$ *as given in* (1) *be any quadrature rule approximating* $\int_a^b f(x)\,dx$, *where* f *is continuous on* $[x_0, x_n]$. *Suppose that* $F' = f$ *and define the polynomials*

$$\Omega(x) := \prod_{j=0}^{n} (x - x_j), \tag{2}$$

$$q_n(x) := \Omega^2(x)\left\{\frac{b-a}{(x-a)(x-b)} - \sum_{j=0}^{n} \frac{\alpha_j}{(x-x_j)^2}\right\}. \tag{3}$$

Then

$$E_n(f) := \int_a^b f(x)\,dx - Q_n(f) = (Fq_n)[x_0, x_0, \ldots, x_n, x_n]. \tag{4}$$

Here, $(Fq_n)[x_0, x_0, \ldots, x_n, x_n]$ is the $(2n+1)$st divided difference of the product Fq_n at the points $x_0, x_0, \ldots, x_n, x_n$. Notice that there are no restrictions on the signs of the weights α_j. Moreover, since some of the weights may be zero, there is no loss of generality in our assumption that the endpoints a, b are nodes of the quadrature formula.

Before embarking on the proof of Theorem 1, we briefly discuss divided differences.

DEFINITION 1. Let $P_m(x) = \sum_{k=0}^{m} a_k x^k$ be the unique polynomial of degree at most m that interpolates (agrees with) the function g at the points $t_0, t_1, \ldots, t_m$. Then the mth divided difference of g in these points is given by

$$g[t_0, \ldots, t_m] := a_m. \tag{5}$$

If $t_0, \ldots, t_m$ are distinct, this definition is unambiguous. In the case that some of the t_j are repeated, we are to understand "interpolating polynomial" in the *Hermite sense*. That is, if t_j is repeated i times, then we mean that the polynomial P_m and its first $i-1$ derivatives agree with g and its first $i-1$ derivatives at t_j.

In the case of distinct t_j, a simple induction yields the familiar recursive definition:

$$g[t_j] = g(t_j), \quad j = 0, \dots, n,$$

$$g[t_0, \dots, t_k] = \frac{g[t_0, \dots, t_{k-1}] - g[t_1, \dots, t_k]}{t_0 - t_k},$$

where k ranges from 1 to n. More important for us is the following known representation theorem for the divided difference of an analytic function (cf. [**2**, §3.6]).

THEOREM 2. *Let $t_0, \dots, t_m$ be $m + 1$ (not necessarily distinct) points, and let C be a simple closed rectifiable curve in the z-plane surrounding $t_0, \dots, t_m$. If g is analytic inside and on C, then*

$$g[t_0, \dots, t_m] = \frac{1}{2\pi i} \int_C \frac{g(z)}{(z - t_0) \cdots (z - t_m)} \, dz. \tag{6}$$

Proof. The representation (6) can be derived from the *Hermite error formula*

$$g(z) - P_m(z) = \frac{1}{2\pi i} \int_C \frac{\omega(z) g(t)}{\omega(t)(t - z)} \, dt, \tag{7}$$

$$\omega(z) := \prod_{j=0}^{m} (z - t_j),$$

for z inside C, where P_m is the interpolating polynomial of Definition 1. Using the Cauchy integral representation for $g(z)$, formula (7) is equivalent to

$$P_m(z) = \frac{1}{2\pi i} \int_C \left[\frac{\omega(z) - \omega(t)}{z - t} \right] \frac{g(t)}{\omega(t)} \, dt. \tag{8}$$

Notice that the right-hand side of (7) vanishes at the points t_j (the zeros of $\omega(z)$) in the Hermite sense, and that the integral in (8) is a polynomial of degree at most m in z. (These two observations show that the right-hand side of (8) is indeed the interpolating polynomial P_m.) Now since

$$\frac{\omega(z) - \omega(t)}{z - t} = z^m + \cdots,$$

we see from (8) that the coefficient a_m of z^m in P_m is just the integral

$$a_m = \frac{1}{2\pi i} \int_C \frac{g(t)}{\omega(t)} \, dt,$$

which verifies formula (6). □

Theorem 2 removes much of the mystery surrounding divided differences with coincident points, and permits a simple proof of Theorem 1. Schneider's proof of

Theorem 1, which makes use of Leibniz's rule for divided differences and other identities, is algebraic in nature. Our proof shows that the result follows in a natural way from the Cauchy Integral Theorem.

The Proof of Theorem 1. First assume that f is analytic on the interval $[x_0, x_n]$; then we can assume f has been analytically continued to an open domain containing $[x_0, x_n]$. Since $\int_a^b f(x)\,dx = F(b) - F(a)$, we have

$$\begin{aligned} E_n(f) &= F(b) - F(a) - \sum_{j=0}^{n} \alpha_j F'(x_j) \\ &= \frac{1}{2\pi i}\int_C \frac{F(z)}{z-b}\,dz - \frac{1}{2\pi i}\int_C \frac{F(z)}{z-a}\,dz - \sum_{j=0}^{n} \alpha_j \frac{1}{2\pi i}\int_C \frac{F(z)}{(z-x_j)^2}\,dz \\ &= \frac{1}{2\pi i}\int_C F(z)\left\{\frac{b-a}{(z-b)(z-a)} - \sum_{j=0}^{n} \frac{\alpha_j}{(z-x_j)^2}\right\} dz, \end{aligned}$$

where C is a suitably chosen contour. Now observe from (2) and (3) that the portion of the integrand in brackets is just $q_n(z)/\Omega^2(z)$. Hence

$$E_n(f) = \frac{1}{2\pi i}\int_C \frac{F(z)q_n(z)}{\Omega^2(z)}\,dz. \tag{9}$$

Since q_n is a polynomial, $F(z)q_n(z)$ is analytic inside and on C and so, by Theorem 2, $E_n(f)$ is the divided difference given in (4). This proves the result for analytic f.

In the general case where f is continuous on $[x_0, x_n]$, we construct the interpolating polynomial p that satisfies

$$p(x_i) = F(x_i), \quad p'(x_i) = f(x_i), \quad i = 0, 1, \ldots, n.$$

Since

$$\int_a^b p'(x)\,dx = p(b) - p(a) = F(b) - F(a) = \int_a^b f(x)\,dx,$$

we see that $E_n(f) = E_n(p')$. Moreover we have

$$(pq_n)[x_0, x_0, \ldots, x_n, x_n] = (Fq_n)[x_0, x_0, \ldots, x_n, x_n]$$

because, in general, $g[x_0, x_0, \ldots, x_n, x_n]$ is a linear combination of the numbers $g(x_0), g'(x_0), \ldots, g(x_n), g'(x_n)$ (see [**1**, p. 12]). Thus, applying the first part of the proof to p', we obtain (4) in the general case. □

We now apply Theorem 1 to the study of precision in quadrature methods.

DEFINITION 2. The quadrature method (1) has *precision m* if it integrates exactly every polynomial of degree m or less, but does not integrate exactly some polynomial of degree $m+1$. That is, for every polynomial p with degree $\leqslant m$, $Q_n(p) = \int_a^b p(x)\,dx$, but $Q_n(x^{m+1}) \neq \int_a^b x^{m+1}\,dx$.

In Theorem 1, the polynomial q_n is of degree at most $2n$. As the next corollary shows, the smaller the precise degree of q_n, the higher is the precision of the quadrature scheme.

COROLLARY 1. *Let* $d := \deg q_n$. *If* $d \leqslant 2n-1$, *then the degree of precision of the quadrature scheme* (1) *is* $2n-d-1$.

Proof. Let P_k be a polynomial of degree k and P_{k+1} be an antiderivative of P_k. Then the product $P_{k+1}q_n$ has degree $k+1+d$. Since

$$E_n(P_k) = (P_{k+1}q_n)[x_0, x_0, \ldots, x_n, x_n],$$

and the jth order divided difference of a polynomial of degree at most $j-1$ is zero*, then $E_n(P_k) = 0$ for $k+1+d \leqslant (2n+1)-1$; that is, for $k \leqslant 2n-d-1$. Hence the method integrates exactly every polynomial of degree $2n-d-1$ or less.

It remains to show that $E_n(x^{2n-d}) \neq 0$. With $F(z) := z^{2n-d+1}$, formula (9) asserts that

$$E_n(x^{2n-d}) = \frac{1}{2\pi i}\int_C \frac{F(z)q_n(z)}{\Omega^2(z)}\,dz, \tag{10}$$

where C can be taken as any circle centered at the origin having sufficiently large radius. Since the integrand in (10) is a rational function with numerator degree $2n+1$ and denominator degree $2n+2$, then (after cancelling common factors) we have, in a neighborhood of infinity,

$$\frac{F(z)q_n(z)}{\Omega^2(z)} = \frac{A_1}{z} + \frac{A_2}{z^2} + \cdots,$$

where $A_1 \neq 0$. Hence, from (10),

$$E_n(x^{2n-d}) = \frac{1}{2\pi i}\int_C \left[\frac{A_1}{z} + \frac{A_2}{z^2} + \cdots\right] dz = A_1 \neq 0. \square$$

We remark that if we say that the quadrature scheme (1) has degree of precision -1 if it will not even integrate constants exactly, then Corollary 1 also holds for $d = 2n$.

The reader is invited to apply Corollary 1 to familiar quadrature formulae such as the trapezoid rule, Simpson's rule, and Gaussian quadrature. For example, Simpson's rule is a special case of (1) where $n = 2$, $\alpha_0 = \alpha_2 = (b-a)/6$, $\alpha_1 = 2(b-a)/3$, $x_0 = a$, $x_1 = (b+a)/2$, and $x_2 = b$. A routine calculation shows that $q_2(x)$ reduces to a constant polynomial ($d = 0$) and so (as is well known) Simpson's rule has precision $2n-d-1 = 4-1 = 3$.

Using the fact (proved by Rolle's theorem) that for smooth functions g and real points t_j,

$$g[t_0, \ldots, t_m] = \frac{g^{(m)}(\mu)}{m!}, \quad \text{for some } \mu \in [\min t_i, \max t_i], \tag{11}$$

we can derive the following representation for the error $E_n(f)$ in (4).

*This is an immediate consequence of Definition 1.

COROLLARY 2. *If* $f \in C^{(2n)}[x_0, x_n]$, *then for some* $\mu \in [x_0, x_n]$,

$$E_n(f) = \frac{1}{(2n+1)!} \sum_{j=0}^{d} \binom{2n+1}{j} q_n^{(j)}(\mu) f^{(2n-j)}(\mu), \tag{12}$$

where $d = \deg q_n$.

Proof. From (4), (11), and Leibniz's rule for differentiation we have

$$\begin{aligned} E_n(f) &= (Fq_n)[x_0, x_0, \ldots, x_n, x_n] = \frac{(Fq_n)^{(2n+1)}(\mu)}{(2n+1)!} \\ &= \frac{1}{(2n+1)!} \sum_{j=0}^{2n+1} \binom{2n+1}{j} q_n^{(j)}(\mu) F^{(2n+1-j)}(\mu) \\ &= \frac{1}{(2n+1)!} \sum_{j=0}^{d} \binom{2n+1}{j} q_n^{(j)}(\mu) f^{(2n-j)}(\mu). \square \end{aligned}$$

We remark that formula (12) can be used to give an alternative proof of Corollary 1, which we previously established without appealing to Rolle's theorem.

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