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Error Bounds for the Evaluation of Integrals by Repeated Gauss-Type Formulae

FRANK STENGER*

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1. Introduction

Procedures for numerical evaluation of integrals have been devised but relatively few methods of obtaining error estimates are available. Among the authors who have previously considered this problem are von MISES [*1*], SARD [*2*] and AHLIN [*12*]. With minor exceptions the procedure of these authors is to express the error as a high order derivitive of the integrand; such an error is not always easy to bound. AHLIN develops a 2-term bound for a double integral using the Newton divided difference polynomial. He also expresses the error in the form of a contour integral, but he does not give any method of bounding this integral.

In this paper we derive four methods of bounding the error

$$E_{m_1,\ldots,m_n}(f) = \int_{a_1}^{b_1}\cdots\int_{a_n}^{b_n} w_1(x^1)\ldots w_n(x^n)\, f(x^1,\ldots,x^n)\, dx^n\ldots dx^1 - \sum_{k_1=1}^{m_1}\cdots\sum_{k_n=1}^{m_n} w_{1,k_1}\ldots w_{n,k_n}\, f(x^1_{k_1},\ldots,x^n_{k_n}) \tag{1.1}$$

of repeated Gauss-type quadrature. The applicability of the various procedures depends upon the properties of f, the weight functions $w_i(x^i)$ and the limits of integration. It is possible that only one, or all of the procedures (each with its merits and disadvantages) can be applied to a particular integral.

In equation (1.1) we assume that $w_i(x^i)\,(x^i)^{2k}$ $(i=1, 2, \ldots, n;\ k=0, 1, 2, \ldots)$ is positive and integrable $(\mathscr{L})$ over the integration strip (a_i, b_i) which may be infinite. The numbers $x^i_{k_i}$ are the zeros of polynomials $p_{i,m_i}(x^i)$ (p_{i,m_i} of degree m_i in x^i) orthonormal over (a_i, b_i) with respect to $w_i(x^i)$, and the w_{i,k_i} are the corresponding Gaussian integration weights. Under the assumptions on $w_i(x^i)$, the zeros $x^i_{k_i}(k_i=1, 2, \ldots, m_i)$ are distinct and located in the open interval (a_i, b_i) and the w_{i,k_i} are all positive.

Let us establish a more concise notation. Let $\boldsymbol{K}(j)$ denote the set of integers $(k_j, k_{j+1}, \ldots, k_n)$, $j=1, 2, \ldots, n$, where each k_i ranges from 1 to m_i. Let $\boldsymbol{R}^n$ be the region of integration in (1.1). We put $\boldsymbol{x}^j = x^1, x^2, \ldots, x^j$, $dV(\boldsymbol{x}^j) = \prod_{i=1}^{j} w_i(x^i)\, dx^i$, $f(\boldsymbol{x}^n) = f(\boldsymbol{x}) = f(\boldsymbol{x}^j, \boldsymbol{y}^{j+1})$, and denote

$$\sum_{s\in\boldsymbol{K}(j)} w^j_s\, f(\boldsymbol{x}^{j-1}, \boldsymbol{y}^j_s) = \sum_{k_j=1}^{m_j}\cdots\sum_{k_n=1}^{m_n} w_{j,k_j}\ldots w_{n,k_n}\, f(\boldsymbol{x}^{j-1}, x^j_{k_j}, \ldots, x^n_{k_n}), \qquad (j=1, 2, \ldots, n).$$

* The work of this paper was done by the author at the University of Alberta in 1965—66.

Whenever there is no confusion, we shall suppress subscripts and superscripts. We shall therefore often write x for x^j, k for k_j, w_k for w_{j,k_j}, $p_m(x)$ for $p_{j,m_j}(x)$, $\boldsymbol{x}$ for $\boldsymbol{x}^n$, $\boldsymbol{y}$ for $\boldsymbol{y}^1$, m for m_j, and $\boldsymbol{m}$ for $m_1, m_2, \ldots, m_n$. Thus the equation (1.1) can be written

$$E_{\boldsymbol{m}}(f) = \int_{\boldsymbol{R}^n} f(\boldsymbol{x})\, dV(\boldsymbol{x}) - \sum_{s \in \boldsymbol{K}(1)} \boldsymbol{w}_s^1 f(\boldsymbol{y}_s). \tag{1.1$'$}$$

It is of course presumed that the integral on the right of (1.1)′ exists. More precisely, this implies that given any $\varepsilon > 0$ there exists a compact subset $\boldsymbol{S}^n$ of $\boldsymbol{R}^n$ such that

$$\int_{\boldsymbol{R}^n - \boldsymbol{S}^n} |f(\boldsymbol{x})|\, dV(\boldsymbol{x}) < \varepsilon \prod_{i=1}^{n} \mu_0^i \tag{1.2}$$

where we define

$$\mu_k^i = \int_a^b w_i(x)\, (x)^k\, dx, \qquad k = 0, 1, 2, \ldots. \tag{1.3}$$

It is convenient, further, to define $\boldsymbol{R}^j = \times\{[a_i, b_i],\ i = 1, 2, \ldots, j\}$ and $\boldsymbol{S}^j = \times\{[c_i, d_i],\ i = 1, 2, \ldots, j\}$ where j ranges from 1 to n, and each interval $[c_i, d_i]$ is a compact subset of $[a_i, b_i]$. Then with

$$N = \max_{\boldsymbol{x} \in \boldsymbol{S}^n} |f(\boldsymbol{x})| \tag{1.4}$$

we assume in addition to (1.2) that

$$\int_{(a_j, b_j) - [c_j, d_j]} w_j(x) \left\{ \max\left[N, \left| x - \frac{c_j + d_j}{2} \right|^{2m_j} \right] \right\} dx < \varepsilon\, \mu_0^j \tag{1.5}$$

One assumption is common to all procedures: we require that f have a bounded $2m_j$'th partial derivative with respect to x^j on $[c_j, d_j]$, $j = 1, 2, \ldots, n$. This assumption suffices for the first of the four procedures. For the remaining procedures we assume that, with x, y real, there is an open set $\mathscr{E}_j$ of complex numbers $\zeta = x + \sqrt{-1}\, y$ enclosing $[c_j, d_j]$ such that, with $\boldsymbol{z}^j = \boldsymbol{x}^{j-1}, \zeta, \boldsymbol{y}^{j+1}$ and $\boldsymbol{C}_j = \boldsymbol{S}^{j-1} \times \mathscr{E}_j \times (\boldsymbol{S}^n - \boldsymbol{S}^j)$ (a Cartesian product), $f(\boldsymbol{z}_j)$ is an analytic function of ζ regular for $\boldsymbol{z}^j \in \boldsymbol{C}_j$.

These latter assumptions extend those of Davis [*3*], McNamee [*4*], Hämmerlin [*5*] and Stenger [*6*] in the one-dimensional case. We combine the procedures of these authors in an attempt to also obtain useful results for the case of repeated Gauss-type formulae.

Although we assume that the limits of integration in (1.1) are fixed, bounded or unbounded points, the results of this paper can also be made to include integrals of the form

$$\int_{\varphi_1}^{\psi_1} \int_{\varphi_2}^{\psi_2} \cdots \int_{\varphi_n}^{\psi_n} g(\boldsymbol{x}^n) \prod_{i=1}^{n} dx^i \tag{1.6}$$

where φ_1 and ψ_1 are constant, and $\varphi_j = \varphi_j(\boldsymbol{x}^{j-1})$, $\psi_j = \psi_j(\boldsymbol{x}^{j-1})$, $j = 2, 3, \ldots, n$, are differentiable and bounded almost everywhere, since [*10*, *12*[1]] the sequence of linear transformations

$$x^i = \frac{\varphi_i + \psi_i}{2} + u^i \frac{(\psi_i - \varphi_i)}{2} \qquad (i = 1, 2, \ldots, n) \tag{1.7}$$

[1] Ahlin [*12*] obtains this result for the $n = 2$ case.

will transform the above integral (1.6) into the integral

$$\int_{-1}^{1} \cdots \int_{-1}^{1} G(\boldsymbol{u}^n)\, J \prod_{i=1}^{n} du^i \tag{1.8}$$

where

$$J = \prod_{i=1}^{n} \left[\frac{\psi_i - \varphi_i}{2}\right] \tag{1.9}$$

and $G = g$ under the transformation (1.7).

2. General Procedure for Extending One-dimensional Bounds

The following procedure due to NIKOL'SKII [*11*] (summarized in [*13*] p. 72—75) enables us to reduce the error of repeated integration to that of bounding the error of single integration.

Define

$$I_j = \int_{S^j} \sum_{s \in K(j+1)} w_s^{j+1} f(\boldsymbol{x}^j, \boldsymbol{y}_s^{j+1})\, dV(\boldsymbol{x}^j), \qquad (j = 0, 1, \ldots, n) \tag{2.1}$$

Here $I_n = \int_{S^n} f(\boldsymbol{x}^n)\, dV(\boldsymbol{x}^n)$, and I_0 is the repeated sum on the right of (1.1). We thus obtain

Theorem 2.1. *Let I_j be defined by equation* (2.1). *Then*

$$E_{\boldsymbol{m}}(f) = I_n - I_0 + r(S^n) = \sum_{j=1}^{n} (I_j - I_{j-1}) + r(S^n). \tag{2.2}$$

In (2.2)

$$r(S^n) = \int_{R^n - S^n} f(\boldsymbol{x}^n)\, dV(\boldsymbol{x}^n) \tag{2.3}$$

and

$$\begin{aligned} I_j - I_{j-1} = \int_{R^{j-1}} \sum_{s \in K(j+1)} w_s^{j+1} \Big\{ \int_{c_j}^{d_j} w_j(x)\, f(\boldsymbol{x}^{j-1}, x, \boldsymbol{y}_s^{j+1})\, dx - \\ - \sum_{k=1}^{m} w_k f(\boldsymbol{x}^{j-1}, x_k, \boldsymbol{y}_s^{j+1}) \Big\}\, dV(\boldsymbol{x}^{j-1}). \end{aligned} \tag{2.4}$$

A bound on $r(S^n)$ is given by (1.2). On inspecting (2.4) we observe that we can apply one-dimensional procedures to bound the quantity in braces on the right of this equation. Moreover, if for each j we can obtain a good bound for the quantity in braces on the right of (2.4), then using (2.2) we can also obtain a good bound on the error $E_{\boldsymbol{m}}(f)$.

Corollary 2.1. *Let*

$$|I_j - I_{j-1}| \leqq B_j(m_j), j = 1, 2, \ldots, n.$$

Then

$$|E_{\boldsymbol{m}}(f)| \leqq \sum_{j=1}^{n} B_j(m_j) + \varepsilon \prod_{i=1}^{n} \mu_0^i \tag{2.5}$$

The above theorem and corollary are of course applicable if the x_{i,k_i} and w_{i,k_i} on the right of (1.1) are not Gaussian zeros and weights, i.e. to any other quadrature scheme.

In the following sections we shall give four different procedures for obtaining $B_j(m_j)$.

3. Functions f with $2m_j$'th Partial Derivative Bounded on $[c_j, d_j]$

The Hermite interpolant polynomial of degree $2m_j - 1$ in x^j (whose coefficients may be functions of $(\boldsymbol{x}^{j-1}, \boldsymbol{y}^{j+1})$), $H_j(x^j)$, satisfies

$$(3.1)\qquad \begin{aligned} H_j(x_k) &= f(\boldsymbol{x}^{j-1}, x_k, \boldsymbol{y}_s^{j+1}) \\ \frac{\partial H_j(x)}{\partial x} &= \frac{\partial f(\boldsymbol{x}^{j-1}, x, \boldsymbol{y}_s^{j+1})}{\partial x} \quad \text{at} \quad x = x_k, \qquad (k = 1, 2, \ldots, m) \end{aligned}$$

also satisfies

$$(3.2)\qquad \begin{aligned} & f(\boldsymbol{x}^{j-1}, x, \boldsymbol{y}_s^{j+1}) - H_j(x) \\ & \quad = \frac{1}{(2m)!} \frac{\partial^{2m}}{(\partial x)^{2m}} f(\boldsymbol{x}^{j-1}, \chi(x), \boldsymbol{y}_s^{j+1})\, \varkappa_m^{-2} [p_m(x)]^2. \end{aligned}$$

In (3.2) $\chi(x)$ lies between the largest and smallest of $x, x_1, \ldots, x_m$, and $\varkappa_m$ is the coefficient of x^m in $p_m(x)$.

It follows that, since Gaussian integration is exact for polynomials of degree $2m - 1$, we have

$$(3.3)\qquad \begin{aligned} & \int_{c_j}^{d_j} w_j(x) f(\boldsymbol{x}^{j-1}, x, \boldsymbol{y}_s^{j+1})\, dx - \sum_{k=1}^{m} w_k f(\boldsymbol{x}^{j-1}, x_k, \boldsymbol{y}_s^{j+1}) \\ & \quad = \frac{\varkappa_m^{-2}}{(2m)!} \frac{\partial^{2m}}{\partial \bar{x}^{2m}} f(\boldsymbol{x}^{j-1}, \bar{x}, \boldsymbol{y}_s^{j+1}) \int_{c_j}^{d_j} w_j(x) [p_m(x)]^2\, dx + \\ & \quad + \int_{[a_j, b_j] - [c_j, d_j]} w_j(x) H_j(x)\, dx \end{aligned}$$

for some $\bar{x} \in [c_j, d_j]$. On combining (3.3) with (1.2), (1.4) and (2.4) we obtain

Theorem 3.1. *Let I_j be defined by* (2.1).
Then $|I_j - I_{j-1}| \leqq B_j(m_j)$, where

$$(3.4)\qquad B_j(m_j) = \left\{ \frac{\varkappa_{j,m_j}^{-2}}{\mu_0^j (2m_j)!} \left[\sup_{\boldsymbol{x}^n \in S^n} \left| \frac{\partial^{2m_j}}{(\partial x^j)^{2m_j}} f(\boldsymbol{x}^n) \right| \right] + \varepsilon_j \right\} \prod_{i=1}^{n} \mu_0^i$$

In (3.4) $0 \leqq \varepsilon_j \leqq \mu_0^j \varepsilon$, *and $\varkappa_{j,m_j}$ is the coefficient of x^{m_j} in $p_{j,m_j}(x)$.*

Constants $\varkappa_{j,m_j}$ for well-known special cases are given in Table 2.

Example[2] *3.1.*

$$\begin{aligned} E_{m_1, m_2}(f) = & \int_{x=0}^{\infty} x^{\alpha} e^{-x} \int_{y=-1}^{1} \sqrt{1 - y^2} \cos(ax + by)\, dy\, dx - \\ & - \sum_{\mu=1}^{m_1} \sum_{\nu=1}^{m_2} w_{1,\mu} w_{2,\nu} \cos(a x_\mu + b y_\nu), \end{aligned}$$

[2] Note that $\cos(ax + by) = \cos(ax)\cos(by) - \sin(ax)\sin(by)$ and we can evaluate the above using $m_1 + m_2$ points instead of $m_1 m_2$.

a and b real and $\alpha > -1$. Here

$$\frac{\varkappa_{1,m_1}^{-2}}{(2m_1)!} = \frac{m_1!\,\Gamma(m_1+\alpha+1)}{(2m_1)!} \sim \sqrt{\pi}\,2^{-2m_1} m_1^{\alpha+\frac{1}{2}}$$

$$\frac{\varkappa_{2,m_2}^{-2}}{(2m_2)!} = \frac{\pi}{(2m_2)!\,2^{2m_2+1}} \sim \frac{\pi^{\frac{1}{2}}}{4} m_2^{-\frac{1}{2}} \left(\frac{e}{4m_2}\right)^{2m_2}$$

Since $\left|\frac{\partial^{2m_1}}{(\partial x)^{2m_1}} \cos(ax+by)\right| \leqq a^{2m_1}$, $\left|\frac{\partial^{2m_2}}{\partial y^{2m_2}} \cos(ax+by)\right| \leqq b^{2m_2}$ in the region of integration, we find, using Corollary 2.1 that

$$|E_{m_1,m_2}(f)| \leqq \frac{\Gamma(\alpha+1)}{2}\pi \left\{\frac{\pi^{\frac{1}{2}}}{\Gamma(\alpha+1)} m_1^{\alpha+\frac{1}{2}} \left(\frac{a}{2}\right)^{2m_1} + \frac{m_2^{-\frac{1}{2}}}{2\pi^{\frac{1}{2}}} \left(\frac{be}{4m_2}\right)^{2m_2}\right\}.$$

Thus, while there is no restriction on b, we require that $|a| < 2$ in order that our bound tend to zero as $m_1 \to \infty$. For example, with $\alpha = 0$, $a = \frac{1}{3}$, $b = 2.45$, $m_1 = 4$, $m_2 = 5$, the above estimate gives $|E_{m_1,m_2}(f)| < 6.7 \times 10^{-6}$. The actual error is 2.6×10^{-6}.

4. Functions $f(z^j)$ Analytic and Real when the Components of z^j are Real

We first note the following Lemma.

Lemma 4.1. *Let u and v be real, let $f(u)$ be real and let $f(u+\sqrt{-1}\,v)$ be regular in the ellipse $\mathscr{E}_\varrho(c,d)$ with center at $\frac{c+d}{2}$, foci at (c,d), major and minor axes $\frac{d-c}{2}a$ and $\frac{d-c}{2}\sqrt{a^2-1}$, respectively, where $a>1$, $\varrho = a+\sqrt{a^2-1}$. Then*

$$\inf_{P_{2m-1}} \left\{\sup_{u\in(c,d)} |f(u) - P_{2m-1}(u)|\right\} < \frac{8}{\pi} M(\varrho)\,\varrho^{-2m} \tag{4.1}$$

where $P_{2m-1}(u)$ is a polynomial of degree $2m-1$ in u, and

$$M(\varrho) = \sup_{u+\sqrt{-1}\,v\in\mathscr{E}_\varrho(c,d)} |Re\,f(u+\sqrt{-1}\,v)|. \tag{4.2}$$

The proof of Lemma 4.1 follows from a result of ACHIESER (see e.g. [8] page 87).

The right hand side of equation (2.4) is a linear functional in f. Furthermore, if we replace c_j, d_j by a_j, b_j respectively, then any polynomial $P_{2m_j-1}(x^j)$ of degree $2m_j-1$ in x^j is in the null space of this functional. In particular, this is the case for the polynomial $P_{2m_j-1}(x^j)$ whose coefficients may be functions of (x^{j-1}, y_s^{j+1}), which minimizes the maximum deviation of $f(x^{j-1}, x^j, y_s^{j+1}) - P_{2m_j-1}(x^j)$ over $[c_j, d_j]$. Thus

$$\begin{aligned} I_j - I_{j-1} = \int_{S^{j-1}} \sum_{s\in K(j+1)} w_s^{j+1} \times \\ \times \left\{\int_{c_j}^{d_j} w_j(x)\,[f(x^{j-1}, x, y_s^{j+1}) - P_{2m_j-1}(x)]\,dx - \sum_{k=1}^{m} w_k\,[f(x^{j-1}, x_k, y_s^{j+1}) - \right. \\ \left. - P_{2m_j-1}(x)]\right\} dV(x^{j-1}) + \varepsilon_j \end{aligned} \tag{4.3}$$

where

$$\varepsilon_j = -\int_{S^{j-1}} \int_{(a_j,b_j)-(c_j,d_j)} \sum_{s\in K(j+1)} w_s^{j+1} P_{2m_j-1}(x)\,dx\,dV(x^{j-1}). \tag{4.4}$$

Using the notations of the introduction, let $\mathscr{E}_j = \mathscr{E}_{\varrho_j}(c_j, d_j)$ where $\mathscr{E}_\varrho(c, d)$ is defined in Lemma 4.1, and let C_j, z^j be defined as in the introduction. Let $f(z^j)$ be a regular function of ζ for $z^j \in C_j$, and define

$$M_j(\varrho_j) = \sup_{z^j \in C_j} |\operatorname{Re} f(z^j)|. \tag{4.5}$$

Let

$$\omega_j = \frac{8}{\pi} \inf_{\varrho} M_j(\varrho)\, \varrho^{-2m_j}. \tag{4.6}$$

Then, by Lemma 4.1 it follows that

$$\inf_{P_{2m_j-1}} \left\{ \sup_{x \in S^n} |f(x) - P_{2m_j-1}(x^j)| \right\} < \omega_j. \tag{4.7}$$

In addition, it follows by comparison with the Chebyshev polynomials[3] $T_m(x)$, that for $x \in [a_j, b_j] - [c_j, d_j]$,

$$|P_{2m_j-1}(x)| < 2^{2m_j-2} \{N + \omega_j\} \left\{ \max \left[1, \left| x - \frac{c_j + d_j}{2} \right|^{2m_j-1} \right] \right\} \tag{4.8}$$

where ω_j is defined in (4.6), and N is defined in (1.4).

We also assume that the strip $[c_j, d_j]$ completely covers the zeros of $p_{j,m_j}(x)$. On combining the above results and using (1.2) we finally obtain

Theorem 4.1. *Let $f(z^j)$ be an analytic function of ζ regular for $z^j \in C_j$, and real when ζ is real. Then $|I_j - I_{j-1}| < B_j(m_j)$ where*

$$B_j(m_j) = (2\omega_j + \varepsilon_j) \prod_{i=1}^{n} \mu_0^i. \tag{4.9}$$

In (4.9) *ω_j is defined in* (4.6), *and*

$$\varepsilon_j \leqq 2^{2m_j-2} (N + \omega_j)\, \varepsilon, \tag{4.10}$$

where N is defined in (1.4).

Example 4.1. Let $c_j = -\alpha$, $d_j = \alpha$, and let

$$\sup_{x^i \in [c_i, d_i],\, i \neq j} |\operatorname{Re} f(x^{j-1}, u + \sqrt{-1}\, v, y^{j+1})| = \varphi(u, v)$$

where $u + \sqrt{-1}\, v \in \mathscr{E}_\varrho(-\alpha, \alpha)$, and where

(i) $\varphi_1(u, v) \leqq M(1 - cv)^{-a}$, $a, c, M > 0$, $0 < v < c^{-1}$;

(ii) $\varphi_2(u, v) \leqq M e^{bv^\lambda}$, $b, \lambda, M > 0$, $0 < v$.

Then it is readily shown by minimization of $\varphi(\alpha u, \alpha v)\, (v + \sqrt{1 + v^2})^{-2m}$ with respect to v that

(i) $\min_{\varrho} \left\{ \max_{u, v \in \mathscr{E}_\varrho} \varphi_1(u, v)\, \varrho^{-2m} \right\} < M \left[\dfrac{2em}{a(1 + k^2)^{\frac{1}{2}}} \right]^a \left[\dfrac{1 + (k^2 + 1)^{\frac{1}{2}}}{k} \right]^{-2m}$;

(ii) $\min_{\varrho} \left\{ \max_{u, v \in \mathscr{E}_\varrho} \varphi_2(u, v)\, \varrho^{-2m} \right\} < M \left[\dfrac{ek\lambda}{2^{\lambda+1} m} \right]^{2m/\lambda}$

where in (i) $k = \alpha c$ and in (ii) $k = b\alpha^\lambda$.

Note that although $\varphi(u, v)$ may be larger along the u axis than along the v axis, we can always bound $\varphi(u, v)$ as a function of v since u and v are constrained

[3] Let $P_m(x)$ be any polynomial of degree m, and put $M = \max_{x \in [-1, 1]} |P_m(x)|$. Then for all $|x| > 1$, $|P_m(x)| \leqq M |T_m(x)|$. Here $T_m(x)$ is defined by $T_m(x) = \cos m\theta$ for $x = \cos\theta$.

to be in the interior of the ellipse $\mathscr{E}_\varrho(-\alpha, \alpha)$.

Example 4.2.

$$\int_{z=-\infty}^{\infty} \int_{y=-1}^{1} \int_{x=-1}^{1} \frac{\sqrt{1-x^2}\, e^{-z^2}}{1+a^2x^2y^2} \operatorname{sech}[c(x+y+z)]\, dx\, dy\, dz$$

where a and c are real. In this example weight functions are $\sqrt{1-x^2}$, 1 and e^{-z^2}; i.e. we assume that Chebyshev-Gauss (with respect to x), Legendre-Gauss (with respect to y) and Hermite-Gauss (with respect to z) integrations will be used. Although both $\operatorname{sech}[c(x+y+z)]$ and $(1+a^2x^2y^2)^{-1}$ have singularities that are functions of the remaining variables when one of the variables is complex, these singularities are uniformly bounded away from the region of integration.

We have $|\operatorname{sech}[c(z+y+u+\sqrt{-1}\,v)]| \leqq \frac{1}{\cos(cv)} \leqq \frac{1}{1-\frac{2}{\pi}cv}$, $0 \leqq v < \frac{\pi}{2c}$, where z, y, u and v are real. We furthermore have $|1+a^2y^2(u+\sqrt{-1}\,v)^2]^{-1}| \leqq \frac{1}{(1-a^2v^2)} \leqq \frac{1}{(1-av)}$, $0 \leqq v \leqq 1$, and therefore

$$\left| \frac{\operatorname{sech}[c(u+\sqrt{-1}\,v)+y+z]}{1+a^2y^2(u+\sqrt{-1}\,v)^2} \right| \leqq \frac{1}{(1-av)\left(1-\frac{2c}{\pi}v\right)}.$$

Assuming e.g. $\frac{a}{c} > \frac{2}{\pi}$, it follows by Example 3.1 above that the minimum of

$$\max_{u,y,z} \left| \frac{\operatorname{sech}[c(u+\sqrt{-1}\,v+y+z)]}{1+a^2y^2(u+\sqrt{-1}\,v)^2} \right| (v+\sqrt{v^2+1})^{-2m}$$

with respect to $v < a^{-1}$ is less than

$$\frac{2me}{(1+a^2)^{\frac{1}{2}}} \left[\frac{1+(a^2+1)^{\frac{1}{2}}}{a}\right]^{-2m} \cdot \frac{a\pi}{a\pi-2c}.$$

Moreover, for α and m large,

$$2\int_{\alpha}^{\infty} e^{-z^2}\, dz < 2\int_{\alpha}^{\infty} e^{-z^2} z^{2m_3}\, dz < \alpha^{2m}\, m_3!\, e^{-\alpha^2}.$$

Thus using

$$\int_{-\infty}^{\infty} e^{-z^2}\, dz = \sqrt{\pi}, \int_{-1}^{1} dy = 2, \int_{-1}^{1} \sqrt{1-x^2}\, dx = \tfrac{1}{2}\pi,$$

substituting in equation (19) (Theorem 1), and setting $m_1 = m_2 = m$, we get

$$(*) \qquad \begin{aligned} E_{m,m,m_3}(f) < {} & \pi^{\frac{3}{2}} \left(\frac{64me}{\pi(1+a^2)^{\frac{1}{2}}}\right)\left(\frac{a\pi}{a\pi-2c}\right)\left\{\frac{(a^2+1)^{\frac{1}{2}}+a}{a}\right\}^{-2m} + \\ & + \frac{32m_3e}{\pi[1+(2\alpha c/\pi)^2]^{\frac{1}{2}}}\left(\frac{[1+(2\alpha c/\pi)^2]^{\frac{1}{2}}+1}{2\alpha c/\pi}\right)^{-2m_3} + \\ & + \pi^{-\frac{1}{2}}\alpha^{2m_3} 2^{2m_3-1} m_3!\, e^{-\alpha^2}. \end{aligned}$$

Let us consider for example, the case $a = 1/3$, $c = 1/10$. We must choose α so that the strip $[-\alpha, \alpha]$ completely covers the zeros of the Hermite polynomial

$H_{m_3}(z)$. Using $m_3 = 7$, we may choose[4] $\alpha = 8$. With $m = 6$, we obtain

$$|E_{6,6,7}(f)| < \pi^{\frac{3}{2}}(6.44 + 3.69 + .16) \times 10^{-7} \cong 5.7 \times 10^{-6}.$$

By actual numerical evaluation, $E_{6,6,7}(f) = 0.8 \times 10^{-8}$.

The slow convergence of the above bound (*) is due to the singularities in the complex plane and does not reflect upon the method. Indeed bounding the $2m_j$'th partial derivative of the integrand would be a formidable task. Nor can the methods of Sections 3,5 and 6 be easily applied to this case, especially for a and c large.

5. Functions $f(z^j)$ Regular in $|\zeta| \leqq 1$, $[a_j, b_j] = [-1, 1]$

The method to be developed in this section is applicable to functions f regular for $z^j = x^{j-1}, \zeta, y^{j+1} \in C_j$ where C_j is defined as in Section 1 and $\mathscr{E}_j = \{\zeta : \zeta$ is complex and $|\zeta| \leqq 1\}$. We assume that $[c_j, d_j]$ covers the zeros of $p_{j,m_j}(x)$ and that $f(z^j)$ has a convergent power series expansion

$$f(z^j) = \sum_{k=0}^{\infty} F_{j,k}(x^{j-1}, y^{j+1})\,\zeta^k, \; z^j \in C_j. \tag{5.1}$$

The bounds we shall obtain are useful whenever we can obtain good bounds on the coefficients $F_{j,k}$ in (5.1).

We define numbers e_k^j (these will in general depend on m_j) by

$$e_k^j = \mu_k^j - \sum_{\ell=1}^{m_j} w_{j,\ell}(x_\ell^j)^k, \qquad k = 0, 1, 2, \ldots. \tag{5.2}$$

That $e_k^j = 0$ for $k = 0, 1, \ldots, 2m_j - 1$ is well-known. In the case when $w_j(x) = w_j(-x)$, $e_{2k+1}^j = 0$ for all integers k, and it is furthermore shown in [6] that

$$\mu_{2k}^j > e_{2k}^j > 0, \qquad k \leqq m_j.$$

Using the above facts and definitions and the notation of Theorem 2.1 we find, after a little manipulation, that $I_j - I_{j-1}$ (equation (2.4) with $c_j = a_j = -1$, $d_j = b_j = 1$) is given by

$$I_j - I_{j-1} = \int_{S^{j-1}} \sum_{s \in K(j+1)} w_s^{j+1} \sum_{k=2m_j}^{\infty} e_k^j F_{j,k}(x^{j-1}, y_s^{j+1})\, dV(x^{j-1}). \tag{5.3}$$

Using Corollary 2.1, we thus have

Theorem 5.1. *If the expansion* (5.1) *converges for* $z^j \in C_j$, *then* $|I_j - I_{j-1}| \leqq B_j(m_j)$ *where*

$$B_j(m_j) = \frac{\nu_j(m_j)}{\mu_0^j} \sum_{k=0}^{\infty} F_{j,k}^* \left(\prod_{i=1}^{n} \mu_0^i \right) \tag{5.4}$$

provided the infinite sum on the right exists. Here

$$F_{j,k}^* = \sup_{x^{j-1} \in S^{j-1},\, y^{j+1} \in (S^n - S^j)} |F_{j,k}(x^{j-1}, y^{j+1})| \tag{5.5}$$

[4] Actually $\alpha = (2m_3)^{\frac{1}{2}}$ suffices. However, our particular choice of α gives us a better bound on the final ε term above.

and

$$v_j(m_j) = \sup_{k=0,1,2,\ldots} \left|e^j_{2m_j+k}\right|. \tag{5.6}$$

Table 1. *Error constants for theorem 5.1.*

	$w(x)=1$	$w(x)=(1-x^2)^{\frac{1}{2}}$	$w(x)=(1-x^2)^{-\frac{1}{2}}$
	$x_{n,k}, w_{n,k}$	$x_{n,k}=\cos\left(\frac{k\pi}{n+1}\right)$	$x_{n,k}=\cos\left[\frac{(2k-1)}{2n}\pi\right]$
	in* [9] p. 916	$w_{n,k}=\frac{\pi}{n+1}\sin^2\left(\frac{k\pi}{k+1}\right)$	$w_{n,k}=\frac{\pi}{n}$
n	$v(n)$	$v(n)$	$v(n)$
2	.21164	.09817 4	.67495
3	.10222	.03988 3	.44001
4	.06101 4	.01965 4	.32799
5	.04051 1	.01118 2	.26158
6	.02886 7	.00697 88	.21761
7	.02161 8	.00464 43	.18634
8	.01679 7	.00324 77	.16294
9	.01343 0	.00236 00	.14477
10	.01098 3	.00176 88	.13026
12	.00773 98	.00106 82	.10850
16	.00443 63	.00047 615	.08134 7

* [9] also contains zeros and weights for other quadrature schemes.

Under the assumptions on $w_j(x)$ the numbers $v_j(m_j)$ always exist and can be computed using equation (5.2). Some of these corresponding to three different $w_j(x)$ are given in Table 1 above.

Example 5.1.

$$E_{m_1,m_2}(f) = \int_{-1}^{1}\int_{-1}^{1} \frac{x^4 y^2 e^{xy}}{\sqrt{1-y^2}}\,dx\,dy - \frac{\pi}{m_1}\sum_{j=1}^{m_1}\sum_{k=1}^{m_2} w_k\, x_j^4\, y_k^2\, e^{x_j y_k}.$$

In this case

$$x^4\, y^2\, e^{xy} = \sum_{k=0}^{\infty} \frac{x^{k+4}\, y^{k+2}}{k!}$$

so that

$$F_{1,2k}(y) = \frac{y^{2k-2}}{(2k-4)!}, \qquad F_{1,2k-1} = 0,$$

and

$$F_{2,2k}(x) = \frac{x^{2k+2}}{(2k-2)!}, \qquad F_{2,2k-1} = 0; \qquad k = 1, 2, 3, \ldots.$$

Hence applying Theorem 4.2 we obtain, using

$$\mu_0^1 = \pi, \qquad \mu_0^2 = 2, \quad \text{and} \quad \sum_{j=m}^{\infty} \frac{1}{j!} \leq \frac{e}{m!},$$

$$0 < E_{m_1,m_2}(f) \leq 2\pi\left[\frac{v_1(m_1)}{\pi}\sum_{k=0}^{\infty}\frac{1}{(2m_1+2k-4)!} + \frac{v_2(m_2)}{2}\sum_{k=0}^{\infty}\frac{1}{(2m_2+2k-2)!}\right]$$

$$\leq \frac{\sqrt{2e}}{\pi} v_1(m_1)\left(\frac{e}{2m_1-4}\right)^{2m_1-3.5} + \frac{\sqrt{e\pi}}{2} v_2(m_2)\left(\frac{e}{2m_2-2}\right)^{2m_2-1.5}.$$

For example, with $m_1 = 6$, $m_2 = 5$ using the above estimate,

$$0 < E_{m_1, m_2}(f) \leqq 6.1 \times 10^{-5}.$$

By numerical integration we find that $E_{m_1, m_2}(f) = 3.9 \times 10^{-8}$.

6. Asymptotic Error Estimates

The method to be described in this section is particularly in the case when $f(z^j)$ is an entire function of ζ, or in the case when $f(z^j)$ has singularities far from the region of integration. It is demonstrated for the case of Gauss-Legendre integration in [4] that singularities of $f(z^j)$ close to the region of integration can also be suitably accounted for in obtaining error estimates. However, in attempting to extend that procedure to higher dimensions, difficulties arise due to the fact that singularities of $f(z^j)$ are, in general, functions of $n-1$ variables.

Let us examine the contour integral

$$J_j = \frac{1}{2\pi\sqrt{-1}} \int_L \frac{w_j(x)\, f(x^{j-1}, \zeta, y_s^{j+1})}{(x-\zeta)\, p_{j,m_j}(\zeta)}\, d\zeta. \tag{6.1}$$

In (6.1) L is the circle with center at the origin and radius $\varrho + \delta = \max(|c_j|, d_j) + \delta$ where δ is a fixed positive number. We assume that $f(x^{j-1}, \zeta, y_s^{j+1})$ is a regular function of ζ for $x^{j-1} \in S^{j-1}$ and $|\zeta| \leqq \varrho + \delta$. It follows from (6.1) that

$$J_j = w_j(x) \left[f(x^{j-1}, x, y_s^{j+1}) - \sum_{k=1}^{m} \frac{p_m(x)\, f(x^{j-1}, x_k, y_s^{j+1})}{(x-x_k)\, p_m'(x_k)} \right]. \tag{6.2}$$

Integrating (6.1) and (6.2) from c_j to d_j and interchanging the order of integration in the repeated real and complex integral, we obtain

$$\begin{aligned} &\int_{a_j}^{b_j} w_j(x)\, f(x^{j-1}, x, y_s^{j+1})\, dx - \sum_{k=1}^{m} w_k f(x^{j-1}, x_k, y_s^{j+1}) \\ &\quad = \frac{1}{2\pi\sqrt{-1}} \int_L f(x^{j-1}, \zeta, y_s^{j+1})\, d\zeta \int_{\alpha_j}^{\beta_j} \frac{w_j(x)\, p_m(x)}{(x-\zeta)\, p_m(\zeta)}\, dx + \varepsilon_j \end{aligned} \tag{6.3}$$

where

$$\varepsilon_j = \int_{(a_j, b_j)-(c_j, d_j)} w_j(x) \left[f(x^{j-1}, x, y_s^{j+1}) - \sum_{k=1}^{m} \frac{f(x^{j-1}, x_k, y_s^{j+1})}{(x-x_k)\, p_m'(x_k)} \right] dx \tag{6.4}$$

and

$$w_k = \int_{a_j}^{b_j} \frac{w_j(x)\, p_m(x)}{(x-x_k)\, p_m'(x_k)}\, dx. \tag{6.5}$$

We now asymptotically approximate the inner integral on the right of (6.3). We assume that $w(x) = O(|x|^r e^{-|x|^\lambda})$ where r and λ are positive numbers. In (6.3), let $\alpha = \max(a, -\varrho)$ and $\beta = \min(b, \varrho)$ where $|\zeta| = \varrho + \delta$ and where δ is a fixed positive number. Thus

$$\begin{aligned} \int_\alpha^\beta \frac{w(x)\, p_m(x)}{(\zeta - x)\, p_m(\zeta)}\, dx &= \frac{1}{\zeta p_m(\zeta)} \int_\alpha^\beta w(x)\, p_m(x) \sum_{k=0}^{m-1} \left(\frac{x}{\zeta}\right)^k dx + \\ &+ \frac{1}{\zeta p_m(\zeta)} \int_\alpha^\beta w(x)\, p_m(x) \left\{ \left(\frac{x}{\zeta}\right)^m + \left(\frac{x}{\zeta}\right)^{m+1} + \frac{(x/\zeta)^{m+1}}{1 - x/\zeta} \right\} dx \end{aligned} \tag{6.6}$$

Under the assumed exponential form of $w(x)$ and the orthogonality property of the polynomials $p_m(x)$, the first integral on the right of (6.6) tends to zero at an exponential rate as $x \to a$ or b, and hence does not contribute towards an asymptotic sequence of the form $\{\zeta^{-k}\}$. Similarly expanding $1/p_m(\zeta)$ in powers of $1/\zeta$,

$$\int_\alpha^\beta \frac{w(x)\,p_m(x)}{\zeta^{m+1}\,p_m(\zeta)}\,dx = \frac{\varkappa_m^{-2}}{\zeta^{2m+1}} + O(|\zeta|^{-2m-2}), \qquad |\zeta| \to \infty, \tag{6.7}$$

where $\varkappa_m$ is the coefficient of x^m in $p_m(x)$. Further,

$$\begin{aligned} &\left| \int_\alpha^\beta \frac{w(x)\,p_m(x)}{\zeta^{m+2}\,p_m(\zeta)} \left\{ x^{m+1} + \frac{x^{m+2}}{\zeta - x} \right\} dx \right| \\ &\qquad \leqq \int_\alpha^\beta w(x) \left| \frac{p_m(x)}{\zeta^{m+2} p_m(\zeta)} \right| \left\{ |x|^{m+1} + \frac{|x|^{m+2}}{\delta} \right\} dx \\ &\qquad = O(|\zeta|^{-2m-2}), \qquad |\zeta| \to \infty. \end{aligned} \tag{6.8}$$

We substitute the above results into equation (6.3) to obtain

Lemma 6.1. *Let $\varkappa_m$ be the coefficient of x^m in $p_m(x)$, and let $w(x) = O(|x|^r\, e^{-|x|^\lambda})$, for both $x \to a$ and $x \to b$, where r and λ are positive numbers. Let L be the contour $|\zeta| = \varrho + \delta$ where δ is a fixed positive number and where, with $\alpha \geqq \max(a, -\varrho)$ and $\beta \leqq \min(b, \varrho)$, ϱ is chosen sufficiently large so that the conditions* (1.2) — (1.5) *are satisfied. Then*

$$\begin{aligned} I_j - I_{j-1} &= \int_{S^{j-1}} \sum_{s \in K(j+1)} w_s^{j+1} \times \\ &\times \frac{1}{2\pi\sqrt{-1}} \int_L f(x^{j-1}, \zeta, y_s^{j+1})\,[1 + O(|\zeta|^{-1})]\,\frac{\varkappa_{j,m_j}^{-2}}{\zeta^{2m_j+1}}\,d\zeta\,dV(x^{j-1}), \qquad |\zeta| \to \infty. \end{aligned} \tag{6.9}$$

In order to obtain an estimate on the bound of the difference $I_j - I_{j-1}$ in (6.9) we again prefer to express $f(x^{j-1}, \zeta, y_s^{j+1})$ as a positive function $M(R)$ of $R = |\zeta|$ which bounds f on the compact set $S^{j-1} \times (S^n - S^j)$. That is, let

$$M(R) = \sup_{x^{j-1} \in S^{j-1},\, |\zeta| = R,\, y^{j+1} \in (S^n - S^j)} |f(x^{j-1}, \zeta, y^{j+1})|. \tag{6.10}$$

On replacing the quantity in square brackets on the right of (6.9) by 1, we obtain an asymptotic estimate on the bound of $I_j - I_{j-1}$.

Theorem 6.1. *Let $M_j(R)$ be defined by* (6.10). *Then $(I_j - I_{j-1}) \leqq B_j(m_j)$ where for large R*

$$B_j(m_j) = \frac{\varkappa_{j,m_j}^{-2}}{\mu_0^j} \left(\prod_{i=1}^n \mu_0^i \right) \frac{M_j(R)}{R^{2m_j}}. \tag{6.11}$$

Example 6.1. Let $M_j(R) \leqq A(1 - cR)^{-a}$ where A, a and c are positive, $0 \leqq R < c^{-1}$. The minimum of $A(1 - cR)^{-a}\, R^{-2m}$ *qua* function of R occurs for $R = c^{-1}\left(1 + \frac{a}{2m}\right)^{-1}$ and is $A\, e^{a^2} \left(\frac{2m}{a}\right)^a c^{2m}$; hence

$$|I_j - I_{j-1}| \leqq \left(\prod_{i=1}^n \mu_0^i \right) \left(\frac{\varkappa_{j,m}^{-2}}{\mu_0^j} \right) A\, e^{a^2} \left(\frac{2m}{a} \right)^a c^{2m}.$$

In the case when the integration strip is bounded (and $c<1$), we can choose m sufficiently large so that the above error estimate is as small as we please. On the other hand, if the range of integration in the jth variable is infinite and f has

Table 2. *Error constants for theorem 6.1*

Weight Function	$(1-x)^\alpha(1+x)^\beta$ $\alpha>-1, \beta>-1$	$x^\alpha e^{-x}$ $\alpha>-1$	e^{-x^2}
Orthogonal Polynomial	Jacobi [interval$(-1, 1)$]	Laguerre [interval $(0, \infty)$]	Hermite [interval $(-\infty, \infty)$]
$\varkappa_{j,n}^{-2}$	$2^{1+\alpha+\beta+2n}\, n! \times \dfrac{\Gamma(1+\alpha+\beta)\, B(1+\alpha+n, 1+\beta+n)^*}{\Gamma(1+\alpha+\beta+2n)}$	$n!\,\Gamma(n+\alpha+1)$	$\dfrac{\pi n!}{2^n}$

* $B(x, y)=\dfrac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}$

complex singularities, R will remain bounded. This implies however, that the largest zero of p_{j,m_j} is to remain bounded, which in turn bounds m_j. In this case, the Gaussian quadrature scheme will not, in general, converge, and as in the case when evaluating a function by its asymptotic expansion, we may find in this case that there is a "best" m_j which minimizes $|I_j-I_{j-1}|$.

Example 6.2. $M_j(R)\leqq A\exp\{bR^\lambda\}$ where A, b and λ are positive. Assuming $w_j(x)=O(e^{-|x|^\beta})$, $x\to a$ or b, where $\beta>\lambda$, all Gaussian quadrature schemes converge in this case. We obtain, taking $R=\left(\dfrac{2m}{b\lambda}\right)^{1/\lambda}$,

$$|I_j-I_{j-1}|\leqq\left(\prod_{i=1}^{n}\mu_0^i\right)\frac{\varkappa_{j,m}^{-2}}{\mu_0^j}A\left(\frac{eb\lambda}{2m}\right)^{2m/\lambda}.$$

Example 6.3. We apply the theory of this section to bound[5]

$$E_{m_1,m_2,m_3}(f)=\int_{x=-\infty}^{\infty}\int_{y=0}^{\infty}\int_{z=-1}^{1}\frac{100\,e^{-y-z^2}J_0(\frac{1}{2}y)\cos z}{x^2-4x+104}\,dx\,dy\,dz$$
$$-100\sum_{k_1=1}^{m_1}\sum_{k_2=1}^{m_2}\sum_{k_3=1}^{m_3}w_{1,k_1}w_{2,k_2}w_{3,k_3}\frac{J_0(\frac{1}{2}y_{k_2})\cos z_{k_3}}{x_{k_1}^2-4x_{k_1}+104}$$

where Gauss-Legendre integration is used with respect to x, Gauss-Leguerre with respect to y, and Gauss-Hermite with respect to z. Thus $\mu_0^1=2$, $\mu_0^2=1$, $\mu_0^3=\sqrt{\pi}$. In the range of integration, $|100/(x^2-4x+104)|\leqq 1$, $|J_0(\frac{1}{2}y)|\leqq 1$ and $|\cos z|\leqq 1$. In the complex plane, $100/[\zeta^2-4\zeta+104]$ has poles at α_1 and α_2 ($\alpha_1=2+10i$, $\alpha_2=2-10i$) where $|\alpha_s|>10$, $s=1, 2$. Hence $M_1(R)\leqq(1-R/10)^{-1}$. $|J_0(\frac{1}{2}\zeta)|\leqq$

[5] Observe that this integral can be evaluated with $m_1+m_2+m_3$ points instead of with $m_1m_2m_3$, by writing it in the form

$$\int_{-\infty}^{\infty}F(z)\,dz\int_{0}^{\infty}G(y)\,dy\int_{-1}^{1}H(x)\,dx.$$

$\left(\frac{1}{\pi R}\right)^{\frac{1}{2}} e^{\frac{1}{2}R}\left[1+O\left(\frac{1}{R}\right)\right] = M_2(R)$ $(|\zeta| = R)$; and $|\cos\zeta| \leqq e^R = M_3(R)$ $(|\zeta| = R)$. Using Table 2 and applying Theorem 6.1, we find that

$$|E_{m_1, m_2, m_3}(f)| \leqq \sum_{j=1}^{3} |I_j - I_{j-1}|$$

$$\leqq 2\pi^{\frac{1}{2}}\left\{\frac{e m_1}{2}\left(\frac{1}{400}\right)^{m_1} + \pi^{\frac{1}{2}} m_2^{\frac{1}{2}}\left(\frac{1}{8}\right)^{m_2} + \sqrt{2}\,\pi\, m_3^{\frac{1}{2}}\left(\frac{e}{8 m_3}\right)^{m_3}\right\}$$

$$\cong 3.54(1.70 + 1.70 + 1.44) \times 10^{-5} \cong 1.7 \times 10^{-4}$$

with $m_1 = 2$, $m_2 = 6$, $m_3 = 5$. The actual error when evaluating the integral by numerical integration formula is 0.8×10^{-5}.

Conclusion

In order to illustrate the four methods of bounding the error of repeated Gauss-type quadrature, we have given an example for each. It is worthwile to observe that it may be possible to apply more than one procedure to a particular integral; the user should choose that procedure which best suits a particular integrand.

Although the procedure of Section 3 is applicable in all cases, it is conveniently applied only to integrands for which high order partial derivatives are easily obtained.

The procedure of Section 4 is applicable to integrals over bounded and unbounded regions. It is applicable only to integrands f which, when considered to be functions of complex variables, are analytic, and real when these variables are real. The sharpness of the error bounds obtained depends on how well we can bound the real part of f in ellipses of complex numbers enclosing the integration strips.

In Section 5 we have given a procedure for integrals over bounded regions symmetric about the origin. For this procedure we require the integrand to be regular in a circle which includes the integration strip. The sharpness of the error bounds depends on how well we can bound the Taylor series coefficients of the integrand.

The procedure of Section 6 is applicable to integrands regular in large circles enclosing the integration strips. Here we obtain not error bounds, but asymptotic estimates on these bounds.

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Department of Mathematics
The University of Michigan
Ann Arbor, Michigan, 48104, USA