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A MODIFIED GAUSSIAN QUADRATURE RULE FOR INTEGRALS INVOLVING POLES OF ANY ORDER

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Abstract.

By applying the theory of completely symmetric functions we derive a Gaussian quadrature rule which generalizes that due to McNamee. A feature of this generalization is the inclusion of an explicit correction term taking account of the presence of poles (of any order) of the integrand close to the integration-interval. A numerical example is provided to illustrate the formulae.

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1. Introduction.

The problem considered is that of evaluating numerically an integral of the form

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

where $[a, b]$ is a finite interval, f is analytic on $[a, b]$ and w may have singularities in $[a, b]$ or at its end-points, but is integrable over $[a, b]$. Since the interval can be transformed by a linear transformation to $[-1, 1]$, we shall take as our standard form

$$I(f) = \int_{-1}^{1} w(x)f(x)dx. \tag{1}$$

We shall assume that f can be continued analytically into some region of the complex plane, but that the resulting complex function has a finite number of poles close to $[-1, 1]$.

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Unlike many previous authors, we concentrate specifically on cases when the poles are of order greater than one. Such multiple poles have also been considered by Lether [3, 4], but our method differs from his in many respects. It was first investigated in Okecha [7], and is based on Gaussian quadrature. It generalizes some results from Hunter [1].

2. The method.

Suppose that in (1) f is analytic on $[-1,1]$, and that it can be continued analytically to give a function which is analytic within and on some contour D in the complex plane, except at a finite number of poles $z_1, z_2, \ldots, z_r$, where z_t is of order m_t $(t = 1, 2, \ldots, r)$. We shall assume that the principal part of the Laurent expansion of f about z_t is

$$\sum_{k=1}^{m_t} \varrho_{tk}(z-z_t)^{-k}, \tag{2}$$

where the values ϱ_{tk} are known.

Our intention here is to describe a method of evaluating $I(f)$ numerically for any values of the multiplicities m_t. Associated with the weight function $w(x)$ there is a sequence of orthogonal polynomials $\{p_0(x), p_1(x), \ldots\}$ satisfying

$$\int_{-1}^{1} w(x)p_m(x)p_n(x)dx = 0 \qquad (m \neq n). \tag{3}$$

We shall denote the zeros of $p_n(x)$ by $x_{n1}, x_{n2}, \ldots, x_{nn}$; provided $w(x) \geqslant 0$ in $[-1, 1]$, these are real and distinct, and lie in the interval $(-1, 1)$.

To develop the numerical method, we consider the contour integral

$$\int_D \frac{f(z)dz}{(z-x)p_n(z)},$$

where x is real, with $-1 < x < 1$, and does not coincide with one of the zeros of $p_n(z)$. The integrand has the following poles:

(i) a simple pole at x, with residue $f(x)/p_n(x)$,

(ii) simple poles at x_{ns}, $(s = 1, 2, \ldots, n)$, with residues

$$\frac{f(x_{ns})}{(x_{ns}-x)p_n'(x_{ns})}, \text{ and}$$

(iii) a pole of order m_t at each of the points z_t $(t = 1, 2, \ldots, r)$. Suppose the residue at z_t is $\delta_t(x)$. To obtain an expression for it, suppose the Taylor series about z_t for $1/p_n(z)$ is

$$1/p_n(z) = \sum_{s=0}^{\infty} H_{ts}(z-z_t)^s. \tag{4}$$

Then

$$f(z)/p_n(z) = \left(\sum_{k=1}^{m_t} \varrho_{tk}(z-z_t)^{-k} + \ldots\right) \sum_{s=0}^{\infty} H_{ts}(z-z_t)^s.$$

The principal part of this expansion is

$$\sum_{j=1}^{m_t} K_{tj}(z-z_t)^{-j}, \tag{5}$$

where

$$K_{tj} = \sum_{k=j}^{m_t} \varrho_{tk} H_{t,\,k-j}. \tag{6}$$

Also,

$$(z-x)^{-1} = -\sum_{j=0}^{\infty} (z-z_t)^j/(x-z_t)^{j+1}. \tag{7}$$

So

$$\frac{f(z)}{(z-x)p_n(z)} = -\left(\sum_{j=1}^{m_t} K_{tj}(z-z_t)^{-j} + \ldots\right) \sum_{k=0}^{\infty} (z-z_t)^k/(x-z_t)^{k+1}.$$

Picking out the term in $(z-z_t)^{-1}$, we get

$$\delta_t(x) = -\sum_{s=1}^{m_t} K_{ts}/(x-z_t)^s. \tag{8}$$

Combining these results,

$$\frac{1}{2\pi i}\int_D \frac{f(z)dz}{p_n(z)(z-x)} = \frac{f(x)}{p_n(x)} + \sum_{s=1}^{n} \frac{f(x_{ns})}{(x_{ns}-x)p_n'(x_{ns})} - \sum_{t=1}^{r}\sum_{s=1}^{m_t} \frac{K_{ts}}{(x-z_t)^s}.$$

Rearranging,

$$f(x) = \sum_{s=1}^{n} \frac{f(x_{ns})p_n(x)}{(x-x_{ns})p_n'(x_{ns})} + \sum_{t=1}^{r}\sum_{s=1}^{m_t} \frac{K_{ts}p_n(x)}{(x-z_t)^s} + \frac{1}{2\pi i}\int_D \frac{f(z)p_n(x)dz}{(z-x)p_n(z)}. \tag{9}$$

Multiplying by $w(x)$ and integrating over $[-1, 1]$, we obtain finally

$$I(f) = G_n + R_n + E_n, \tag{10}$$

where

$$G_n = \sum_{s=1}^{n} w_s f(x_{ns}), \tag{11}$$

with

$$w_s = \int_{-1}^{1} \frac{w(x)p_n(x)dx}{(x-x_{ns})p_n'(x_{ns})} \tag{12}$$

is the standard Gaussian quadrature approximation to $I(f)$;

$$R_n = \sum_{t=1}^{r} \sum_{s=1}^{m_t} (-1)^s K_{ts} q_{ns}(z_t), \tag{13}$$

where

$$q_{ns}(z) = \int_{-1}^{1} \frac{w(x)p_n(x)dx}{(z-x)^s}, \qquad (z \notin [-1,1]); \tag{14}$$

and

$$E_n = \frac{1}{2\pi i} \int_D \frac{f(z)q_{n1}(z)dz}{p_n(z)}. \tag{15}$$

Equation (10) is the basis of the method suggested for evaluating $I(f)$. The term R_n will be regarded as a correction to be added to the standard Gaussian approximation G_n; E_n then gives the error in the corrected approximation. McNamee's results [5] correspond to the case $R_n = 0$.

The main difficulty in applying this method lies in the evaluation of the correction term R_n. For each pole z_t, we must carry out four steps:

(i) determine the coefficients H_{ts} of eqn (4);
(ii) determine the coefficients K_{tj} using eqn (6);
(iii) evaluate the functions $q_{ns}(z_t)$ of eqn (14);
(iv) evaluate the term given by the inner sum in (13).

Of these, steps (i) and (iii) are the most difficult. We shall consider them separately in the next two sections.

Before doing so, it is worthwhile pointing out that if f is a real function, the poles z_t will occur in conjugate pairs, and it is then necessary to evaluate the terms in (13) corresponding to poles above the real axis only, as the corresponding terms for poles below the real axis will be their conjugates.

3. Evaluation of H_{ts}.

Denoting by a_n the coefficients of z^n in the expansion of $p_n(z)$, we have

$$\begin{aligned} 1/p_n(z) &= a_n^{-1} \prod_{s=1}^{n} (z-x_{ns})^{-1} \\ &= a_n^{-1} \prod_{s=1}^{n} (z_t - x_{ns})^{-1} \prod_{k=1}^{n} \left(1 - \frac{z-z_t}{x_{nk}-z_t}\right)^{-1} \\ &= \frac{1}{p_n(z_t)} \sum_{s=0}^{\infty} h_s(u_1, u_2, \ldots, u_n)(z-z_t)^s, \end{aligned} \tag{16}$$

where

$$u_k = 1/(x_{nk} - z_t), \qquad (k = 1, 2, \ldots, n) \tag{17}$$

and $h_s(u_1, u_2, \ldots, u_n)$ is the *completely symmetric function* or *homogeneous product sum of degree* s in $u_1, u_2, \ldots, u_n$, (see Littlewood [2]. Chapter V). Thus

$$H_{ts} = h_s(u_1, u_2, \ldots, u_n)/p_n(z_t). \tag{18}$$

Now for any $j \leqslant n$, the functions $h_s(u_1, u_2, \ldots, u_j)$ are generated by the formula

$$\prod_{k=1}^{j} (1-u_k t)^{-1} = \sum_{s=0}^{\infty} h_s(u_1, u_2, \ldots, u_j) t^s.$$

Multiplying by $(1-u_j t)$ and equating terms in t^s we obtain, after some manipulation, the recurrence relation

$$h_s(u_1, u_2, \ldots, u_j) = h_s(u_1, u_2, \ldots, u_{j-1}) + u_j h_{s-1}(u_1, u_2, \ldots, u_j). \tag{19}$$

This can be used to generate $h_s(u_1, u_2, \ldots, u_j)$ for $s = 1, 2, \ldots, m_t - 1$ and $j = 0, 1, \ldots, n$, from the initial values

$$\left.\begin{array}{ll} h_0(u_1, u_2, \ldots, u_j) = 1, & (j \geqslant 0) \\ h_s(\phi) = 0 \quad , & (s > 0) \end{array}\right\} \tag{20}$$

where ϕ is the empty set (corresponding to the value $j = 0$).

If $w(x)$ is an even function, the zeros x_{nk} are symmetrically distributed about 0, and we can exploit this symmetry by introducing them in pairs in generating $h_s(u_1, u_2, \ldots, u_n)$. If $x_{n,j-1} = -x_{nj}$, equation (19) can be replaced by

$$\begin{aligned} h_s(u_1, \ldots, u_j) = {} & h_s(u_1, u_2, \ldots, u_{j-2}) \\ & + [2z_t h_{s-1}(u_1, u_2, \ldots, u_j) + h_{s-2}(u_1, u_2, \ldots, u_j)]/(x_{nj}^2 - z_t^2). \end{aligned} \tag{21}$$

4. Evaluation of the functions $q_{ns}(z)$.

The orthogonal polynomials $p_n(x)$ satisfy a recurrence relation of the form

$$p_{n+1}(x) = (A_n x - B_n) p_n(x) - C_n p_{n-1}(x), \qquad (n \geqslant 0) \tag{22}$$

with $p_0(x) = a_0$ (constant), $p_{-1}(x) = 0$. From (14) and (22), we readily deduce that

$$q_{n+1,s}(z) = (A_n z - B_n) q_{ns}(z) - C_n q_{n-1,s}(z) - A_n q_{n,s-1}(z), \quad (s \geqslant 1, n \geqslant 0), \tag{23}$$

the initial values being given by the equations

$$q_{n0}(z) = \begin{cases} a_0 \int_{-1}^{1} w(x) dx, & (n = 0) \\ 0 \quad , & (n > 0) \end{cases} \tag{24}$$

$$q_{-1,s}(z) = 0, \qquad (s \geqslant 0).$$

The above recurrence relations can be used to generate the functions $q_{ns}(z)$, provided analytical expressions for $q_{0s}(z)$ are known. In many cases, these can be obtained directly from (14); alternatively, once

$$q_{01}(z) = a_0 \int_{-1}^{1} \frac{w(x)dx}{z-x} \tag{25}$$

has been determined, we can obtain expressions for $q_{0s}(z)$ by repeated use of the formula

$$q_{n,s+1}(z) = -q'_{ns}(z)/s, \qquad (s \geq 1), \tag{26}$$

with $n = 0$.

It is useful, perhaps, to give a few special cases here.

(i) If $w(x) = 1$, we have

$$q_{0s}(z) = \begin{cases} 2Q_0(z) = \ln((z+1)/(z-1)) \quad , & (s = 1) \\ [(z-1)^{1-s} - (z+1)^{1-s}]/(s-1), & (s > 1). \end{cases}$$

(ii) If $w(x) = (1-x^2)^{-1/2}$, we have

$$q_{01}(z) = \pi/(z^2-1)^{1/2}.$$

Expressions for $q_{0s}(z)$ for $s > 1$ can then be obtained by using (26).

If $|z|$ is small, the recurrence relations (23) can be used in the forward direction in both n and s. Otherwise, they are unstable in the forward direction, and a modification of Miller's backward algorithm [6] must be used. This can be obtained by rewriting (23) as a set of simultaneous equations. In matrix form, these are

$$A\boldsymbol{q}^{(s)} = \boldsymbol{b}^{(s)} \tag{27}$$

where

$$A = \begin{bmatrix} (A_1z-B_1) & -1 & 0 & 0\ldots\ldots \\ -C_2 & (A_2z-B_2) & -1 & 0\ldots\ldots \\ 0 & -C_3 & (A_3z-B_3) & -1\ldots\ldots \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \end{bmatrix}$$

$$\boldsymbol{q}^{(s)} = [q_{1s}(z) \quad q_{2s}(z) \quad q_{3s}(z)\ldots]^T$$

$$\boldsymbol{b}^{(s)} = [(c_1q_{0s}(z)+A_1q_{1,s-1}(z)) \quad A_2q_{2,s-1}(z) \quad A_3q_{3,s-1}(z)\ldots]^T, \quad (s \geq 1).$$

If we truncate the system (27) to N simultaneous equations for some suitable $N > n$, we can solve them by triangular decomposition for $s = 1, 2, \ldots, m_t$ in turn; this is equivalent to applying the recurrence relation in the forward direction in s, but backwards in n. As usual with such methods, the determination of the appropriate value of N is a problem. We shall not pursue it further here; in many cases, z_t will be small enough to enable us to use (23) in the forward direction. This point will be discussed further in the next section.

5. Discussion and example.

The method described in the foregoing sections of this paper can be quite effective. However, it requires a certain amount of analytical work in determining the Laurent coefficients ϱ_{tk}, and also involves an appreciable amount of complex arithmetic. For these reasons, it is perhaps best used only in cases where some of the poles z_t are sufficiently close to the interval $[-1, 1]$ to have a serious effect on standard quadrature methods.

These points can be illustrated by using the example

$$F(a) = \int_{-1}^{1} \frac{e^x dx}{(x^2+a^2)^3} = \int_{-1}^{1} \frac{\cosh x dx}{(x^2+a^2)^3}, \qquad (a > 0). \tag{28}$$

The integrand has poles of order 3 at the points $\pm ia$. For the second form of the integral, the Laurent coefficients at $z_1 = ia$ are given by the equations

$$\varrho_{11} = i(\cos a - 3\sin a/a - 3\cos a/a^2)/16a^3$$
$$\varrho_{12} = -(2\sin a + 3\cos a/a)/16a^3$$
$$\varrho_{13} = i\cos a/8a^3.$$

When $a = 1$, our method, with $n = 4$, gave the values $G_4 = 1.1778839$, $R_4 = 0.0131268$, leading to the value $F(1) = 1.1910108$, which is correct to 7 decimal places. However, as the same accuracy can be obtained by using 16-point Gaussian quadrature or by, e.g., composite 4-point Gaussian quadrature, with the interval $[-1, 1]$ subdivided into 5 equal sub-intervals, it is questionable whether the extra work involved in our method is worthwhile.

On the other hand, when $a = 0.1$, the situation is very different. The results are given in the following table.

Evaluation of $F(0.1)$

n	G_n	R_n	G_n+R_n
2	57.885267	117947.88	118005.77
4	699.18325	117306.58	118005.77
8	8903.1293	109102.64	118005.77
12	29819.129	88186.636	118005.77
16	55828.944	62176.822	118005.77

Surprisingly, 8-digit accuracy is obtained, in this case, with $n = 2$. To obtain comparable accuracy using Gaussian quadrature without the correction term, a value of about 100 is required for n.

In this example, since the two poles of the integrand lie on the imaginary axis, it is possible to avoid the use of complex arithmetic by working with the *real* qantities $i^{-n}p_n(ia)$, $i^{s-n}q_{ns}(ia)$ and $i^{-s}h_s(u_1, u_2, \ldots, u_n)$; as to the last of these, we have

$$h_0(u_1, u_2, \ldots, u_n) = 1$$

$$i^{-1}h_1(u_1, u_2, \ldots, u_n) = \begin{cases} 2\displaystyle\sum_{j=1}^{n/2} \frac{a}{x_{nj}^2 + a^2} , & (n \text{ even}) \\ \dfrac{1}{a} + 2 \displaystyle\sum_{j=1}^{(n-1)/2} \frac{a}{x_{nj}^2 + a^2}, & (n \text{ odd}) \end{cases}$$

where in each case the summation is over the positive zeros x_{nj}. The value of $i^{-2}h_2(u_1, u_2, \ldots, u_n)$ is then obtained by applying equation (21).

The considerations of the last paragraph will not apply in the case of poles off the imaginary axis. However in many cases we shall be able to get round this difficulty as follows. Suppose for simplicity that $w(x) = 1$ and that there is just one conjugate pair of poles $z_1 = \alpha + i\beta$, $z_2 = \alpha - i\beta$, where $\beta > 0$ is small. If α is inside the interval $[-1, 1]$ and not too near one of its end-points we can subdivide $[-1, 1]$ into two or more subintervals, of which one is centred on α. We then apply the methods of this paper to the subinterval centred on α only; the contributions from the other subintervals will be less severely affected by the poles, and can be evaluated by Gaussian quadrature. A further advantage of this approach is that, once the subinterval centred on α has been transformed to $[-1, 1]$, the poles will in many cases be close to 0, so that the recurrence relation (23) can be used in the forward direction.

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