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ESTIMATION OF ERROR IN APPROXIMATE NUMERICAL INTEGRATION NEAR A SIMPLE POLE USING CHEBYSHEV POINTS

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INTRODUCTION

In problems of physical interest there often occur definite integrals in which the integrands may have a simple pole within the region of integration. Quadrature formula for such integrals were given by Opitz (1961) representing a part of the integrand by a Lagrangian interpolation polynomial over arbitrary nodes. Basu (1971) used Chebyshev nodes of the first kind to obtain an expression for approximate integration, but did not discuss the error estimate. Recently in a paper accepted for publication, Kundu (1977) has discussed quadrature formula without the error term in presence of a simple pole in terms of Chebyshev nodes of the second kind. In this note, we give a quadrature formula in terms of Chebyshev nodes of the second kind in a form which is less sensitive to round off errors and which consumes less computer time. This formula has the added advantage of remaining valid even if the pole approaches a node. This, however, is not the case with Basu's formula which is subject to the implicit restriction that the pole is different from the nodes.

In our discussion we also give error estimates of the problems of Basu and Kundu. These error estimates have been tested against specific examples and found to predict the magnitudes of actual errors with appreciable precision. It is also found that the Chebyshev nodes of both the kinds have the same power of producing equally precise quadrature formulas when the number of nodes is not very small; but for small number of nodes, points of the second kind offer a greater promise for accuracy than points of the first kind.

THEORY

Let us consider the integral $\int_a^b f(x)\,\mathrm{d}x$ in which the integrand $f(x)$ has the form

$$f(x) = \frac{g(x)}{P - x} \tag{1}$$

where $g(x)$ is a regular function in $[a, b]$ which does not vanish at a specified point $P(a < P < b)$. Without any loss of generality we may take $a = -1$, $b = 1$. Here and elsewhere the value of an improper integral means its principal value.

To obtain a quadrature formula suitable for the above type of integrals, we replace $g(x)$ by a Lagrange interpolation formula on the set of Chebyshev points of the second kind

$$x_k = \cos \frac{k\pi}{n+2}, \quad k = 1, 2, \ldots, n+1 . \tag{2}$$

Points x_k are the zeros of the $(n+1)$-degree Chebyshev polynomial $U_{n+1}(x)$ of the second kind defined by

$$U_{n+1}(x) = \sin[(n+2)\,\theta]/\sin\theta , \quad x = \cos\theta . \tag{3}$$

Effecting the necessary change in the integral under consideration, we can write

$$\int_{-1}^{1} f(x)\,dx = I + E \tag{4}$$

where

$$I \equiv \sum_{r=1}^{n+1} \frac{g_r}{U'_{n+1}(x_r)} \int_{-1}^{1} \frac{U_{n+1}(x)\,dx}{(x - x_r)(P - x)}, \tag{5}$$

$$E \equiv \int_{-1}^{1} \frac{U_{n+1}(x)}{2^{n+1}} \frac{g(x, x_1, \ldots, x_{n+1})}{(P - x)}\,dx .$$

In the last integral $g(x, x_1, \ldots, x_{n+1})$ denotes a divided difference of order $(n+1$ of $g(x)$.

Now

$$U_n(x_r)\,U'_{n+1}(x_r) = \frac{n+2}{\sin^2\theta_r}, \quad r = 1(1)\,n+1 \tag{6}$$

where

$$\theta_r = \frac{r\pi}{n+2}$$

and by the Christoffel-Darboux relation for orthogonal polynomials [Isaacson and Keller, p. 205],

$$\frac{U_{n+1}(x)}{x - x_r} = \frac{2}{U_n(x_r)} \sum_{j=0}^{n} U_j(x_r)\,U_j(x) . \tag{7}$$

Through these relations we can write

$$I = \sum_{r=1}^{n+1} \frac{2g_r \sin^2\theta_r}{n+2} \sum_{j=0}^{n} U_j(x_r) \int_{-1}^{1} \frac{U_j(x)\,dx}{P - x} . \tag{8}$$

Further, using the relations

$$(9) \qquad \int_{-1}^{1} U_n(x)\,\mathrm{d}x = \frac{1 + (-1)^n}{n+1},$$

$$\sum_{j=0}^{n} U_j(x_r)\, U_j(x) = \sum_{j=0}^{n-1} A_j\, U_j(x)\,(p - x) + C$$

where A and C are constants to be determined by the conditions

$$(10) \qquad PA_j - \tfrac{1}{2}A_{j-1} - \tfrac{1}{2}A_{j+1} + C\delta_{0j} = U_j(x_r), \quad j = 0(1)\,n$$

$$A_j = 0, \quad j < 0 \quad \text{or} \quad j \geqq n,$$

we can finally write

$$(11) \qquad I = \sum_{r=1}^{n+1} \frac{2g_r \sin^2 \theta_r}{n+2} \left(\sum_{j=0}^{(n-1)/2} \frac{2A_{2j}}{2j+1} + C \log\left(\frac{1+P}{1-P}\right)\right)$$

where $[x]$ means the integral part of x.

Approximation (11) has the advantage over the approximations suggested by Basu (1971) and Kundu (1978) in that it can be applied even when 'P' coincides with a node; moreover, it consumes less computer time for its evaluation than the other two.

Again through the relation

$$(12) \qquad U_j(x) = 2x\, U_{j-1}(x) - U_{j-2}(x),$$

we can write

$$(13) \qquad \lambda_j - 2p\lambda_{j-1} + \lambda_{j-2} = \frac{2}{j}\{(-1)^j - 1\}, \quad j = 1, 2, \ldots, n+1$$

where

$$(14) \qquad \lambda_j = \int_{-1}^{1} \frac{U_j(x)}{P - x}\,\mathrm{d}x.$$

Since $U_{-1}(x) \equiv 0$ and $\lambda_0 = \log(1 + P)/(1 - P)$, λ_j can be recursively calculated by (13) for a positive integer j. This provides another way of computing the value of I by formula (8) and this value may be used as a check for the approximation (11). However, as a quadrature formula, (8) with equation (13) is as powerful as the formula (10) with equation (11). We suggest the use of the pair (8) and (13) in place of the pair (10) and (11); for, it can be associated with a sharp theoretical error estimate which can be easily evaluated along with it.

ERROR ESTIMATE

The error E in the approximation $\int_{-1}^{1} f(x)\,\mathrm{d}x \simeq I$ is given by the second member of (5). The integrand of E contains a divided difference of $g(x)$ which is not in general known and so evaluation of E is not in general possible. However, it is possible to deduce bounds for E from (5). We first write the integral for E in the form

$$E = -\frac{1}{2^{n+1}} \int_{-1}^{1} g(x, P, x_1, \ldots, x_{n+1})\, U_{n+1}(x) + \tag{15}$$

$$+ \frac{1}{2^{n+1}}\, g(P, x_1, \ldots, x_{n+1}) \int_{-1}^{1} \frac{U_{n+1}(x)}{P - x}\,.$$

Now it is known that

$$g(x, x_1, \ldots, x_m) = g^{(m)}(\xi)/m! \tag{16}$$

where ξ is a point lying between the smallest and the largest of the points $x, x_1, \ldots, x_m$. Using (16) in (15) we get

$$E = -\frac{1}{2^{n+1}(n+2)!} \int_{-1}^{1} g^{(n+2)}(\xi)\, U_{n+1}(x)\, \mathrm{d}x + \tag{17}$$

$$+ \frac{1}{2^{n+1}(n+1)!}\, g^{(n+1)}(\eta) \int_{-1}^{1} (U_{n+1}(x)/(P - x))\, \mathrm{d}x$$

where ξ and η are some points in the obvious intervals. Since for $x \in [-1, 1]$

$$|U_{n+1}(x)| \leqq n + 2\,,$$

it follows from (17) that

$$|E| \leqq \frac{M}{2^{n+1}(n+1)!}\, [2 + |\lambda_{n+1}|] \tag{18}$$

where

$$M \equiv \max_{x \in [-1,1]} \{|g^{(n+1)}(x)|, |g^{(n+2)}(x)|\}\,.$$

The error bound (18) is suitable in case one computes I by (8) using the recursive relation (13). If, however, one computes I by (11), then the use of (18) involves wastage of some extra time. Inequality (18) needs then to be replaced by an other suitable form which avoids the use of the recursion (13). This can be achieved through the use of a Markoff (1916) inequality. If $P_n(x)$ is a polynomial of degree n and

$$L \equiv \max_{x \in [a,b]} |P_n(x)|$$

then for $x \in [a, b]$,

$$|P_n^{(k)}(x)| \leqq \frac{L\, 2^{2k} k!\, n}{(b - a)^k\, (n + k)} \binom{n + k}{n - k}\,. \tag{19}$$

Now

$$U'_{n+1}(x) = \frac{1}{n+2} T''_{n+2}(x),$$

where $T_{n+2}(x)$ is the $(n+2)$nd degree Chebyshev polynomial of the first kind.

Hence estimating $U'_{n+1}(x)$ by the inequality (19) we get

$$|U'_{n+1}| \leqq \frac{(n+1)(n+2)(n+3)}{3}. \tag{20}$$

Now for some point ξ between x and P we can write

$$\lambda_{n+1} = \int_{-1}^{1} \frac{U_{n+1}(P) + (x - P) U'_{n+1}(\xi)}{P - x} dx$$

and so

$$\begin{aligned} |\lambda_{n+1}| &\leqq |\lambda_0 U_{n+1}(P)| + \tfrac{2}{3}(n+1)(n+2)(n+3) \leqq \\ &\leqq (n+2)|\lambda_0| + \tfrac{2}{3}(n+1)(n+2)(n+3). \end{aligned} \tag{21}$$

Using (21) in (18) we finally get

$$|E| \leqq \frac{M}{2^{n+1}(n+1)!} [2 + (n+2)|\lambda_0| + \tfrac{2}{3}(n+1)(n+2)(n+3)]. \tag{22}$$

The error estimate (22) can be used with the formulas (10) and (11). It is to be noted that the estimate (22) is much inferior to (18) for small values of n. Fot M not too large, formula (22) can be used for moderate to large values of n.

ERROR ESTIMATE IN BASU'S CASE

Following Basu (1971), if we used the zeros of the $(n+1)$st Chebyshev polynomial $T_{n+1}(x)$ of the first kind in place of the zeros of $U_{n+1}(x)$ as the nodes of integration, then the error of approximation would be given by

$$E_T = \frac{1}{2^n} \int_{-1}^{1} \frac{T_{n+1}(x) g(x, x_0, \ldots, x_n)}{P - x}. \tag{23}$$

Since $|T'_{n+1}(x)| \leqq (n+1)^2$, proceeding as in the first case we would get

$$|E_T| \leqq \frac{M}{2^n(n+1)!} \left[\frac{2}{n+2} + |\mu_{n+1}| \right] \tag{24}$$

where

$$\mu_{n+1} \equiv \int_{-1}^{1} \frac{T_{n+1}(x) dx}{P - x};$$

clearly

$$\mu_0 = \log\left(\frac{1+P}{1-P}\right),$$

$$\mu_1 = \mu_{-1} = P\mu_0 - 2$$

and

$$\begin{aligned} \mu_{j+1} - 2P\mu_j + \mu_{j-1} &= 4/(j^2 - 1) \quad \text{for} \quad j \text{ even}, \\ &= 0 \qquad\qquad\quad \text{for} \quad j \text{ odd}, \end{aligned}$$

$$j = 1, 2, \ldots, n.$$

A cruder version of (24) is

$$(25) \qquad |E_T| \leqq \frac{M}{2^n(n+1)!}\left[\frac{2}{n+2} + 2(n+1)^2 + |\lambda_0|\right].$$

Inequality (24) gives a tighter bound for E than inequality (18). The quadrature formula pair equations (8) and (13) or (10) and (11) is valid for all P such that $|P| < 1$. The accuracy of the formula grows rapidly and steadily with n if the nodes are different from P. However, it can be seen from the annexed table for small n that the speed of convergence is affected when P is equal to or close to a node. This situation also arises and is little more pronounced for the quadrature formula based on the first kind of points. In identical situation, the use of the second kind of nodes results in a greater speed of convergence than the use of the first set, at least for small values of n. This is understandable in the light of the fact that the polynomials $U_n(x)$ are solutions of a best approximation problem in the space $L_1[-1, 1]$ [Achieser, p. 81].

NUMERICAL EXAMPLE

We now take $g = e^x$ for numerical purpose. Computed values of the integral and error estimates are given in the table for a few arbitrary values of P and various values of n.

In the table I, $|E|$ and $|E|'$ have the following meaning:

I_1 = value of I computed by using formulas (8) and (13);

I_2 = value of I computed by using Basu's formula properly adjusted to accomodate for a 'P' equal or nearly equal to a node;

$|E_i|$ = magnitude of actual error in I_i;

$|E_i|'$ = error bound predicted by formula (18) for $i = 1$ and by (24) for $i = 2$.

From the table we see that accuracies of the computed values grow steadily and rapidly with n when P is not a node or very close to a node. This can be seen for $P = -0{\cdot}2$. In this case for every given value of n, approximation I_1 is better than the approximation I_2 but $|E_2|'$ is a sharper bound for $|E_2|$ than $|E_1|'$ for $|E_1|$. The table also shows the damping effect of the closeness of P to a node on the growth of accuracy of computed values. Let us consider, for example, $P = 0{\cdot}0$. In this case for every even n, P is a node of both $U_{n+1}(x)$ and $T_{n+1}(x)$. Within the desired degree of accuracy we see that an even number of nodes produces a better result than the next higher odd number of nodes. For $P = -0{\cdot}9$, U_5, U_6 and U_7 each have a zero close to P. They are, respectively, $-0{\cdot}866$, $-0{\cdot}901$ and $-0{\cdot}923$. This fact (together with

TABLE

n	P	I_1	$\|E_1\|$	$\|E_1\|'$	I_2	$\|E_2\|$	$\|E_2\|'$
	·59	−·34598332	·002	·02	−·35914091	·01	·03
3		−·34888278	·0007	·003	−·35008754	·002	·005
4		−·34824470	·00009	·0003	−·34826206	·0001	·0003
5		−·34816091	·000002	·00001	−·34815671	·000002	·000007
6		−·34815852	·0000002	·000001	−·34815814	·0000006	·000002
7		−·34815869	·00000004	·0000001	−·34815868	·00000005	·00000009
8		−·34815869	·00000004	·0000000	−·34815873	·00000000	·00000000
9		−·34815873	·00000000				
10							
3	0	−2·1142840	·0002	·01	−2·1146502	·0002	·006
4		−2·1135750	·0009	·004	−2·1128575	·002	·005
5		−2·1145008	·0000009	·0001	−2·1145021	·0000004	·00003
6		−2·1145063	·000005	·00002	−2·1145110	·000009	·00003
7		−2·1145017	·0000000	·0000005	−2·1145017	·0000000	·0000001
8							
9							
10							
3	−·2	−2·2467431	·007	·03	−2·2420161	·01	·04
4		−2·2533280	·0004	·002	−2·2528804	·0008	·003
5		−2·2537796	·00007	·0003	−2·2538382	·0001	·0004
6		−2·2537104	·0000008	·00001	−2·2537127	·000002	·000007
7		−2·2537107	·0000003	·000001	−2·2537104	·0000008	·000002
8		−2·2537110	·0000000	·00000005	−2·2537110	·0000000	·00000003
9		−2·2537110		·00000000	−2·2537110		·00000000
3	−·9	−2·6223685	·01	·06	−2·6214314	·01	·04
4		−2·6069451	·002	·007	−2·6078035	·001	·004
5		−2·6089741	·0002	·0006	−2·6088558	·00005	·0002
6		−2·6087993	·00002	·00004	−2·6088107	·0000005	·000004
7		−2·6088106	·0000005	·000002	−2·6088099	·0000003	·0000009
8		−2·6088101	·0000000	·00000006	−2·6088102	·0000001	·00000008
9							

the proximity of the boundary $x = -1$) explains the initial low speed of convergence of I_1. But here the agreement between the actual and predicated error bounds is remarkable.

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Souhrn

ODHAD CHYBY PŘI PŘIBLIŽNÉ NUMERICKÉ INTEGRACI V BLÍZKOSTI JEDNODUCHÉHO PÓLU S POUŽITÍM ČEBYŠEVOVÝCH BODŮ

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V článku je odvozena kvadraturní formule s odhadem chyby pro funkce s jednoduchým pólem. Jako uzly integrace jsou použity Čebyševovy body druhého druhu.

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