

QUADRATURE OF INTEGRANDS WITH A LOGARITHMIC SINGULARITY

JOHN A. CROW

ABSTRACT. A quadrature rule is presented that is exact for integrands of the form $\pi(\xi) + \varpi(\xi) \log \xi$ on the interval $(0, 1)$, where π and ϖ are polynomials. The computed weights and abscissae are given for one- through seven-point rules. In particular, the four-point rule is exact for integral operators with logarithmically singular kernel on a cubic B-spline basis, and it is expected these results shall prove useful for numerical applications of weighted-residual finite element methods.

1. INTRODUCTION

In the formulation of solutions to initial value and boundary value problems for a partial differential equation by means of integral operators, one is led in a natural way to integrals with singular kernel functions. This is due to the singularity of the associated fundamental solution and the fact that this fundamental solution, or some derivative of it, often is used for the kernel of the integral representation. The problems arising in mathematical physics in two spatial dimensions typically lead to kernels with a logarithmic singularity. For example, the wave equation $\Psi_{tt} = c^2 \Delta \Psi$ is reduced by the form $\Psi(t, \xi) = \psi(\xi) e^{-i\omega t}$ to the Helmholtz equation $\Delta \psi + k^2 \psi = 0$, where $k^2 = \omega^2/c^2$ and $\xi \in R^2$, and which in two dimensions has a fundamental solution involving $H_0^{(1)}(k|\xi|)$.

In numerical work based upon an integral representation with such a kernel, these integrals pose a bit of a problem for typically, as in a Galerkin method solution, many numerical integrals are required, but only particular ones (the so-called *self-terms*) possess a truly singular kernel and special handling of these terms must be performed. For the sake of concreteness, consider for the moment integrals of the form $\int_0^1 f(\xi) d\xi$ where f has a weak, integrable singularity at the lower endpoint. Two straightforward ways of computing such an integral are: (1) Replacing the lower endpoint by ε (> 0), and computing the resulting integrals for a sequence of ε 's tending to zero, perhaps employing some sort of sequence extrapolation; and (2) decomposing f into an easily-treated singular part f_s of special form and a bounded part f_b such that $f = f_s + f_b$, then computing the individual integrals by special techniques and

Received by the editor October 28, 1991.

1991 *Mathematics Subject Classification.* Primary 65D30, 65D32.

Key words and phrases. Numerical integration, quadrature formula, Galerkin method.

TABLE 1

N	Abcissae	Weights
0	0.36787 94411 71442 32159 55237 70161 (-0)	0.10000 00000 00000 00000 00000 00000 (+1)
1	0.88296 86513 76530 11759 59513 85185 (-1)	0.29849 98937 05524 91470 84741 43289 (-0)
	0.67518 64909 09887 20103 62743 16962 (-0)	0.70150 01062 94475 08529 15258 56711 (-0)
2	0.28811 66253 09518 31174 32844 63059 (-1)	0.10333 07079 64928 64676 92515 92664 (-0)
	0.30406 37296 12137 65261 08623 58639 (-0)	0.45463 65259 70098 70884 06911 21425 (-0)
	0.81166 92253 44078 11686 37051 77761 (-0)	0.44203 27660 64972 64439 00572 85911 (-0)
3	0.11802 59099 78449 18264 91730 11095 (-1)	0.43391 02877 84143 91101 89836 96321 (-1)
	0.14282 56799 77483 69513 68513 69176 (-0)	0.24045 20976 59460 67597 84500 61567 (-0)
	0.48920 15226 54574 47871 90313 05699 (-0)	0.42140 34522 59775 93197 88150 24211 (-0)
	0.87867 99740 69183 70280 76889 06265 (-0)	0.29475 34213 02349 00094 08365 44590 (-0)
4	0.56522 28205 08009 71359 27256 19673 (-2)	0.21046 94579 18546 29119 00268 26421 (-1)
	0.73430 37174 26522 73406 15889 38883 (-1)	0.13070 55407 44446 69759 10762 54992 (-0)
	0.28495 74044 62558 15371 45276 01926 (-0)	0.28970 23016 71314 15684 15903 51057 (-0)
	0.61948 22640 84778 38140 68089 43051 (-0)	0.35022 03701 20398 71028 55468 04135 (-0)
	0.91575 80830 04698 33378 46091 80928 (-0)	0.20832 48416 71985 80616 27839 07174 (-0)
5	0.30258 02137 54625 87097 29970 37526 (-2)	0.11351 33881 72726 09440 49112 38284 (-1)
	0.40978 25415 59506 15053 46596 31089 (-1)	0.75241 06995 49165 22917 35628 91092 (-1)
	0.17086 32955 26877 29472 51498 29786 (-0)	0.18879 00416 15416 35460 95079 43772 (-0)
	0.41325 57088 44793 24766 64814 55164 (-0)	0.28582 07218 27227 31198 66834 80085 (-0)
	0.70909 51467 90628 54395 00459 17084 (-0)	0.28448 64278 91408 80004 51516 69844 (-0)
	0.93823 95903 77167 09135 50205 94716 (-0)	0.15431 03998 93758 40100 08094 93362 (-0)
6	0.17596 52118 46577 42805 62642 84949 (-2)	0.66326 66319 02570 51178 39049 89051 (-2)
	0.24469 65071 25133 67427 64533 73497 (-1)	0.45799 70797 84753 34125 57673 48120 (-1)
	0.10674 80568 58788 95418 02597 81083 (-0)	0.12384 02080 71318 19455 04895 64922 (-0)
	0.27580 76412 95917 38307 78595 12057 (-0)	0.21210 19260 23811 93010 79148 75456 (-0)
	0.51785 51421 51833 71615 86689 61982 (-0)	0.26139 06456 72007 72564 65806 06859 (-0)
	0.77181 54853 62384 90027 46468 69494 (-0)	0.23163 61802 90909 38431 88155 26104 (-0)
	0.95284 13405 81090 55899 43065 88503 (-0)	0.11859 86656 44451 72613 27836 41957 (-0)

summing the results. A simple example in which the latter approach might be applicable is seen in the evaluation of

$$\int_0^h H_0^{(1)}(k\xi)[a + b\xi + c\xi^2] d\xi$$

as the integrand naturally separates into a part which is well-behaved (f_b) and another part which is a power series attached to a logarithm (f_s). Other methods include change-of-variable techniques [2, 4, 6, 7, 11] (the tanh, erf, and IMT rules), Gaussian quadrature for specialized singular weight functions [10], or most simply computing and ignoring the singularity. Evidently there are relative strengths and weaknesses associated with these approaches.

In this paper we describe a quadrature rule suited for integrands with and without logarithmic singularities. In particular, this rule

$$(1) \quad \int_0^1 f(\xi) d\xi = \sum_{n=0}^N w_n f(x_n) + \mathfrak{R}_{N+1}(f)$$

is exact ($\mathfrak{R}_{N+1}(f) = 0$) for every f of the form

$$(2) \quad f(\xi) = \pi(\xi) + \varpi(\xi) \log \xi$$

in which π and ϖ are polynomials of degree at most N . Thus, the interest lies in being able to compute numerically integrals, possibly possessing a logarithmic singularity in their integrands, without having to develop special methods for handling them or separating them from the nonsingular ones. The approach

taken is similar in spirit to the one by Harris and Evans [5], appending singular basis functions to the usual (polynomial) quadrature basis. It is hoped that rules of this type will be found useful in computations in which a weakly singular integral operator is acting upon smooth functions as in the case when a spline basis is assumed in the Galerkin method. Low-order weights and abscissae ($N = 0, \dots, 6$) are presented in Table 1. In applications of the finite element method, these low-order rules perhaps are the ones most useful.

2. DERIVATION OF THE WEIGHTS AND ABSCISSAE

Let \mathfrak{P}_N be the linear space of polynomials on $[0, 1]$ of degree at most N . We shall require a quadrature rule of the type (1) exact for every f of the form (2) with $\pi, \varpi \in \mathfrak{P}_N$. Explicitly, we need

$$\sum_{n=0}^N w_n [\pi(x_n) + \varpi(x_n) \log x_n] = \int_0^1 [\pi(\xi) + \varpi(\xi) \log \xi] d\xi,$$

for every $\pi, \varpi \in \mathfrak{P}_N$. In particular, the choices $\varpi = 0$ and $\pi = 0$ lead alternately to the separate requirements

$$\sum_{n=0}^N w_n \pi(x_n) = \int_0^1 \pi(\xi) d\xi$$

and

$$\sum_{n=0}^N w_n \varpi(x_n) \log x_n = \int_0^1 \varpi(\xi) \log \xi d\xi$$

for each $\pi, \varpi \in \mathfrak{P}_N$. These must then hold for each basis function of \mathfrak{P}_N . A natural basis to select is from the set of power functions on $[0, 1]$ and this choice leads to a Vandermonde system of equations; it is unfortunate though, that such systems are notorious for being ill-conditioned. When the numerical solution method to be described was used with this basis, condition numbers of this matrix varied quite a bit with estimates of $10^8 - 10^{15}$ being typical for the case $N = 4$ prior to convergence. A more judicious choice is the shifted Legendre polynomials, $P_\nu^*(\xi) = P_\nu(2\xi - 1)$ [1]. There are two reasons for selecting these polynomials: First, they are orthogonal on $[0, 1]$ and this ought to help in the conditioning of the problem; and second, all required integrals may be evaluated analytically and in a simple fashion. Then we must have for $\nu = 0, \dots, N$,

$$\sum_{n=0}^N w_n P_\nu^*(x_n) = \int_0^1 P_\nu^*(\xi) d\xi$$

and

$$\sum_{n=0}^N w_n P_\nu^*(x_n) \log x_n = \int_0^1 P_\nu^*(\xi) \log \xi d\xi.$$

Upon evaluating the integrals (the final one is obtained from 2.17.8.2 of [8]) we obtain the following nonlinear system of $2N+2$ equations in $2N+2$ unknowns

satisfied by the quadrature weights and abscissae:

$$(3) \quad \sum_{n=0}^N w_n P_\nu^*(x_n) = \delta_{0,\nu},$$

$$(4) \quad \sum_{n=0}^N w_n P_\nu^*(x_n) \log x_n = g_\nu,$$

for every $\nu = 0, \dots, N$. Here, $g_0 = -1$ and $g_\nu = (-1)^{1+\nu}/\nu(1+\nu)$ for $\nu = 1, \dots, N$. Numerical solution of this system, at least for the small N of interest in applications of the finite element method, has been effected by iteration. For every $X = (X_0, \dots, X_N) \in R^{N+1}$, let $A(X)$ be the linear operator associated with the matrix of elements $A_{ij}(X) = P_i^*(X_j)$. Then (3) and (4) are of the form

$$A(x)w = d, \quad A(x)v(x, w) = g,$$

where $v_i(x, w) = w_i \log x_i$ and x and w are the required abscissae and weights. Clearly, if we know the solution values of w and v , the weights and abscissae are determined since $x_i = \exp(v_i/w_i)$. A one-step iteration is suggested naturally by the linearized system

$$A(X)W = d, \quad A(X)v(X', W) = g,$$

where here we regard X as an estimate of the abscissae and X' a refinement of this estimate. We have $W = A(X)^{-1}d$ and $v(X', W) = A(X)^{-1}g$ so that the iteration is well defined for every invertible $A(X)$. In this way we have an iteration of the general form $X' = \varphi(X)$.

3. NUMERICAL RESULTS

Clearly, if the iteration $X' = \varphi(X)$ converges and the resulting $A(X)$ is nonsingular, then we have the desired quadrature rule; but it is unfortunate that in practice these iterates bounce about quite a bit— φ is not a contraction. It was found though that the operator $A_\mu : R^{N+1} \rightarrow R^{N+1}$ with $A_\mu X = X + \mu(\varphi(X) - X)$ tends to be contractive for $\mu \approx 1/2$. The resulting convergence is very slow (it appeared to be at most linear) but useful for providing starting values for a Newton-Raphson scheme for $F_\mu(x) = 0$ with F_μ defined by $F_\mu(X) = (I - A_\mu)X$. A real problem for higher N was obtaining reasonable estimates for the abscissae to begin the iteration, and the resulting convergence, or lack thereof, was rather sensitive to this initial choice; this sensitivity increases with increasing N and suggests the need for using some sort of continuation method.

All computations were performed using about 50 significant decimal digits with the aid of Smith's FM multiple precision software [9]. The computed weights and abscissae to 30S are given in Table 1; they have been checked and are believed to be accurate to all shown places.

4. COMMENTS

The set of integrands of the form (2) has the nice property that it is closed under scaling of the interval, for, if $f = \pi + \varpi \log$, then

$$\begin{aligned} f(h\xi) &= \pi(h\xi) + \varpi(h\xi) \log(h\xi) \\ &= (\pi(h\xi) + \varpi(h\xi) \log(h)) + \varpi(h\xi) \log(\xi), \end{aligned}$$

which also is of the form (2). And since the quadrature rule presented evaluates $\int_0^1 f(\xi) d\xi$ exactly, it also evaluates $\int_0^h f(\xi) d\xi$ exactly, which is a property not shared by most weighted Gaussian quadrature rules. This property makes the rule described attractive for applications in which weakly singular integrals must be evaluated over decreasing or partitioned meshes. It would be useful to establish the Kronrod-Patterson rules associated with the presented quadrature formulas.

BIBLIOGRAPHY

1. M. Abramowitz and I. A. Stegun (eds.), *Handbook of mathematical functions*, ninth printing, Dover, New York, 1965.
2. V. U. Aihie and G. A. Evans, *Variable transformation methods and their use in general and singular quadratures*, Internat. J. Comput. Math. **27** (1989), 91–101.
3. H. Engels and U. Eckhardt, *Algorithm 33: Wilf-quadrature*, Computing **18** (1977), 271–279.
4. G. A. Evans, R. C. Forbes, and J. Hyslop, *The tanh transformation for singular integrals*, Internat. J. Comput. Math. **5** (1984), 339–358.
5. C. G. Harris and W. A. B. Evans, *Extension of numerical quadrature formulae to cater for end point singular behaviours over finite intervals*, Internat. J. Comput. Math. (B) **6** (1977), 219–227.
6. M. Iri, S. Moriguti, and Y. Takasawa, *On a certain quadrature formula*, J. Comput. Math. **17** (1987), 3–20.
7. K. Murota and M. Iri, *Parameter tuning and repeated application of the IMT-type transformation in numerical quadrature*, Numer. Math. **38** (1982), 347–363.
8. A. P. Prudnikov, Yu. A. Brychkov, and O. I. Marichev, *Integrals and series*, vol. 2, *Special functions*, Gordon and Breach, New York, 1986.
9. D. M. Smith, *Algorithm 693: A FORTRAN package for floating-point multiple-precision arithmetic*, ACM Trans. Math. Software **17** (1991), 273–283.
10. A. H. Stroud and D. Secrest, *Gaussian quadrature formulas*, Prentice-Hall, Englewood Cliffs, NJ, 1966.
11. H. Takahasi and M. Mori, *Quadrature formulas obtained by variable transformations*, Numer. Math. **21** (1973), 206–219.
12. H. S. Wilf, *Exactness conditions in numerical quadrature*, Numer. Math. **6** (1964), 315–319.

AUTONETICS MARINE AND AIRCRAFT SYSTEMS DIVISION, ROCKWELL INTERNATIONAL CORPORATION, 3370 MIRALOMA AVENUE, ANAHEIM, CA 92803