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A Comparison of Some Quadrature Methods for Approximating Cauchy Principal Value Integrals

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Cauchy principal value integrals are evaluated by the IMT quadrature scheme, which like the TANH quadrature scheme is essentially a trapezoidal scheme, after making a transformation of the variable of integration. Numerical results for some test problems demonstrate that the IMT scheme is superior to the TANH scheme, while both these methods are comparable to, or even better than, the standard methods like the Gaussian or the Chebyshev schemes, in terms of accuracy and simplicity. © 1995 Academic Press, Inc.

1. INTRODUCTION

The numerical evaluation of Cauchy principal value (CPV) integrals like

$$I(y) = \int_a^b \frac{\phi(x)\,dx}{(x-y)} = \underset{\varepsilon \to 0}{Lt} \left[\int_a^{y-\varepsilon} + \int_{y+\varepsilon}^b \right] \frac{\phi(x)\,dx}{(x-y)}; \quad y \in (a,b), \tag{1}$$

is encountered in many areas like the crack problems in plane elasticity, the singular eigenfunction method in neutron transport, and the airfoil theory. The function $\phi(x)$ is assumed to be Hölder continuous [1] which ensures the existence of the integral. One usually writes the above integral as

$$I(y) = \int_a^b \frac{\phi(x) - \phi(y)}{(x-y)}\,dx + \phi(y) \log\left(\frac{b-y}{y-a}\right) \tag{2}$$

which reduces the task to the evaluation of the weakly singular integral which is the first term of Eq. (2).

There are two widely used numerical schemes for the evaluation of the improper integral. One is the Gauss–Legendre or the Gauss–Jacobi quadrature [2–4] and the other is the Chebyshev quadrature [5–7]. Both schemes are of interpolatory type. However, interpolation is only implicit in the Gaussian scheme. In the Chebyshev scheme, the function $\phi(x)$ is approximated by Chebyshev series expansion for which the coefficients need to be evaluated explicitly.

One of the drawbacks of the Gaussian scheme is that the accuracy of the result is seriously affected by numerical instabilities that arise whenever the singular point (y) happens to fall too close to one of the quadrature nodes. No such difficulty arises in the Chebyshev scheme, since the improper integral can be evaluated in closed form if both $\phi(x)$ and $\phi(y)$ are approximated by the same series. On the other hand, the Chebyshev scheme shows poor convergence whenever the function $\phi(x)$ has singularities of the form $(1-x)^{-\alpha}\,(1+x)^{-\beta}$ with $\alpha, \beta \neq \frac{1}{2}$ and $0 < \alpha, \beta < 1$. In the Gauss–Jacobi scheme, these singular factors are absorbed into the weight function, leaving only the smooth part of the function for the polynomial approximation. This results in better convergence in such situations.

There are some drawbacks common to both schemes. The computational labour is somewhat intensive. In the Gaussian scheme, it arises in the generation of the nodes and the weights which change with each α and β. In the Chebyshev quadrature, the majority of the work is spent on computing the expansion coefficients by fast Fourier transform technique or its equivalents.

The accuracy of both the schemes will be greatly impaired when poles of the integrand lie close to the line of integration [8, 9]. All the abovementioned drawbacks are neatly eliminated in the TANH and the IMT schemes [10–14] which are essentially trapezoidal schemes after a change of variable has been effected. We assume that the range is $(-1, 1)$ in the subsequent discussion since any finite range can always be scaled to $(-1, 1)$.

2. THE TANH SCHEME

The TANH scheme also known as the Sinc scheme is as follows: The variable of integration $x \in [-1, 1]$ is changed to $u \in (-\infty, \infty)$, according to

$$x = \tanh(u); \quad y = \tanh(\bar{u});$$

transforming the CPV integral in (1.1) as

$$I(y) = \int_{-\infty}^{\infty} \frac{\phi[\tanh(u)]\,\text{sech}^2 u\,du}{(\tanh u - \tanh \bar{u})} \tag{1}$$

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The transformed integral is then evaluated by the trapezoidal rule choosing a set of nodes $\{u_k\}$ spaced at intervals h. For the sake of convenience in computation, the sum is written in terms of the original variable itself as

$$I(y) \simeq h \sum_k \phi(x_k) \frac{(1 - x_k^2)}{(x_k - y)}, \quad (2)$$

where $x_k = \tanh(u_k)$ and $k = 0, \pm 1, \pm 2, \ldots$.

The nodes $\{u_k\}$ are prescribed so as to be symmetric with respect to the transformed singular point $\bar{u}$ [14], i.e.,

$$u_k = \bar{u} + (k + \tfrac{1}{2})h. \quad (3)$$

This circumvents the numerical instability associated with the denominator tending to zero while approaching the singular point too closely. The labour involved in computing the nodes x_k for each value of y can be reduced by a bit of algebraic manipulation. We define the nodes

$$z_k = \tanh[(k + \tfrac{1}{2})h], \quad k = 0, \pm 1, \pm 2, \ldots,$$

and accordingly rewrite

$$x_k = (z_k + y)/(1 + yz_k),$$

$$(1 - x_k^2)/(x_k - y) = \frac{(1 - z_k^2)}{z_k(1 + yz_k)} = \frac{1}{z_k} - x_k$$

and

$$I(y) \simeq h \sum_k \phi(x_k) [\frac{1}{z_k} - x_k]. \quad (4)$$

The nodes $\{z_k\}$ need to be computed once only.

Bialecki [15] has developed an alternative Sinc-type formula for the evaluation of CPV integrals which has been shown to be uniformly convergent, independent of the value of y. This scheme as applied to the interval $(-1, 1)$ is

$$x_k = \tanh(kh); \quad y = \tanh(\bar{u}) \quad (5)$$

$$W_k(y) = (1 - x_k^2)\left[1 - (-1)^k \cos\left(\frac{\pi \bar{u}}{h}\right)\right] \quad (6)$$

$$I(y) \simeq h \sum_{k=-N}^{N} \frac{\phi(x_k)}{(x_k - y)} W_k(y). \quad (7)$$

Suitability of the scheme for any y comes from the fact that $w_k(y)$ tends to zero if y approaches some node x_k.

If the nodes are prescribed according to Eq. (5), Eq. (6), and Eq. (7) above, the scheme becomes identical to the TANH scheme. Computational economy and accuracy of the scheme are similar to those of TANH rule and, therefore, this scheme is not considered separately here. These remarks are equally applicable to yet another scheme developed by Bialecki, known as the Sinc–Hunter quadrature rule [16].

3. THE IMT SCHEME

The IMT scheme is analogous to the TANH scheme. Here, the variable is transformed according to

$$x = \frac{1}{Q_0} \int_0^u Q(t)\, dt; \quad u \in [0, 1], \quad (1)$$

where $Q(t) = \exp(-1/t(1 - t))$ and $Q_0 = \int_0^1 Q(t)\, dt$.

The scheme has been used for regular integrals having integrable singularities at the ends of the range of integration. The nodes selected are

$$u_k = k/N, \quad k = 1, 2, \ldots, N - 1,$$

This is not appropriate for CPV integrals. Instead, we adopt from the TANH scheme

$$u_k = \bar{u} + (k - 1/2)/N, \quad k = -m, -m + 1, \ldots, 0, \ldots, n - 1,$$

where $\bar{u}$ is such that

$$y = \frac{1}{Q_0} \int_0^{\bar{u}} Q(t)\, dt \quad (2)$$

and m and n are such that

$$u_{-m-1} \leq 0 \leq u_{-m}, \quad u_{n-1} < 1 \leq u_n.$$

After finding m and n, set $u_{-m-1} = 0$ and $u_n = +1$. With these prescriptions, the CPV integral can be approximated by the sum

$$I(y) \simeq \frac{1}{Q_0} \sum_{k=-m}^{n-1} \frac{\phi(x_k)}{(x_k - y)} \frac{Q(u_k)}{2} [u_{k+1} - u_{k-1}], \quad (3)$$

where x_k corresponds to the node u_k. Note that the interval between nodes $[u_{k+1} - u_{k-1}]$ is uniform except at the end points.

The presence of the poles near the line of integration which can ruin the accuracy of Gaussian and Chebyshev schemes is made harmless by a proper choice of step size. The error in the trapezoidal rule contributed by a pole near the line of integration is known from classical literature, as pointed out by McNamee. He and Schwartz [8, 9] have discussed the problem more recently and show this error to be $O(e^{-2\pi d/h})$, where d is the distance of the nearest singularity of the integrand from the line of integration and h is step size for integration. Step sizes of $d/6$ or smaller are adequate for machine precision

TABLE I

Problem 1: $I = \int_{-1}^{1} \exp[a(t-1)]dt/(t-c)$

a	c	QUADPACK	T H T	TANH	IMT
4	0.5	25(10)	18(10)	128(10)	80(11)
4	0.5	25(11)	18(11)	128(11)	80(11)
4	0.95	25(11)	18(11)	128(11)	80(11)
8	0.2	105(13)	26(13)	160(13)	80(13)
8	0.5	105(13)	26(13)	144(13)	96(13)
8	0.95	65(13)	26(13)	128(9)	64(9)
16	0.2	105(13)	34(13)	176(12)	96(12)
16	0.5	145(13)	34(13)	160(13)	80(13)
16	0.95	105(13)	34(13)	160(13)	96(11)

TABLE III

Problem 3: $I = \int_{-1}^{1} \cos(2\pi at)\, dt/(t-c)$

a	c	QUADPACK	T H T	TANH	IMT
8	0.6	495(12)	66(13)	208(4)	80(13)
8	0.8	425(12)	66(13)	224(5)	80(13)
8	0.95	505(12)	66(13)	284(4)	64(13)
16	0.6	875(13)	98(13)	—	80(13)
16	0.8	785(11)	98(14)	—	80(13)
16	0.95	975(12)	98(14)	—	80(13)
32	0.6	1615(12)	162(14)	—	128(13)
32	0.8	1405(12)	162(14)	—	128(13)
32	0.95	1595(13)	162(14)	—	128(13)

limited accuracy of 14 digits. Numerical experience shows that this restriction is needed only in the vicinity of the pole. If the range of integration is split such that the real part of the pole lies at an end point, the natural accumulation of nodes towards the end in these schemes can take care of step size restrictions automatically. This has been successfully tested by us in many cases.

Here, it should be remarked that an effective and straightforward procedure to remove the undesirable influence of poles has been described by Bialecki [17] with respect to Sinc-type quadrature rules. However, such a procedure does not seem feasible in the case of the IMT rule since the contour integration techniques used in such analysis cannot be directly applied here because of the essential singularity contained in $\exp(-1/t(1-t))$.

4. RESULTS AND DISCUSSIONS

In Ref. [7] five test problems were studied and the number of summations N required to achieve the given accuracy for the integral by the Chebyshev and QUADPACK schemes were indicated for various values of c and a, the point of integral evaluation and the parameter of the integrand, respectively. Here for the same set of test problems we compare the reported accuracies of the Chebyshev scheme and QUADPACK package with those of TANH and IMT schemes. Due to the precision limitations of the machine at our disposal, we are not always able to compare with the highest accuracy values reported in [7]. In such cases, the N values required for the nearest possible accuracy are given and are indicated accordingly. If the integrand is smooth and if the poles of the integrand are far from the line of integration then the Chebyshev scheme is computationally the most economical one. This is indicated in the case of problem 1 (Table I) and problem 3 (Table III). But whenever the poles of the integrand are pretty close to the line of integration the TANH and IMT schemes have a clear superiority over the other two methods. This is illustrated in problems 2 and 4. In problem 2 (Table II) with the pole at 0.125 we need 258 and 208 points for the Chebyshev and IMT schemes at c = 0.95. In problem 4 (Table IV) when the pole is at 1.001 we need 395(12), 642(13), 96(12), and 96(12) points for the QUADPACK, Chebyshev, TANH, and IMT schemes, respectively, with the numbers within the brackets in all the tables denote the number of significant digits and the blank entries indicate the lack of convergence. The entries under column T H T correspond to the Chebyshev scheme indicating the

TABLE II

Problem 2: $I = \int_{-1}^{1} dt/(t^2 + a^2)(t-c)$

a	c	QUADPACK	T H T	TANH	IMT
1	0.2	65(13)	34(13)	192(11)	64(11)
1	0.5	65(13)	34(13)	192(12)	64(12)
1	0.95	65(13)	34(13)	192(12)	80(12)
0.25	0.2	365(12)	130(13)	—	96(12)
0.25	0.5	325(12)	130(13)	—	96(12)
0.25	0.95	235(12)	130(13)	—	96(12)
0.125	0.2	505(11)	258(12)	—	176(11)
0.125	0.5	445(12)	258(13)	—	192(12)
0.125	0.95	325(11)	258(13)	—	208(13)

TABLE IV

Problem 4: $I = \int_{-1}^{1} (1-a^2)\, dt/(1-2at+a^2)(t-c)$

a	c	QUADPACK	T H T	TANH	IMT
0.8	0.15	195(13)	130(12)	96(13)	96(13)
0.8	0.45	205(12)	130(12)	112(13)	96(13)
0.8	0.95	305(12)	130(11)	96(11)	80(11)
0.9	0.15	255(13)	258(11)	112(13)	96(13)
0.9	0.45	265(13)	258(11)	96(12)	96(13)
0.9	0.95	335(12)	258(10)	96(11)	80(11)
0.95	0.15	315(13)	642(15)	96(10)	96(13)
0.95	0.45	325(13)	642(13)	96(12)	80(12)
0.95	0.95	395(12)	642(13)	96(12)	96(12)

TABLE V

Problem 5: $I = \int_0^1 \sqrt{1 - t^2}\, dt/(t - c)$

c	QUADPACK	T H T	TANH	IMT
0.6	315(9)	1026(7)	112(13)	64(13)
0.9	405(9)	1026(6)	96(13)	80(13)
0.95	445(9)	1026(6)	112(13)	80(13)

number of digits of accuracy. In the case of problem 5 (Table V), where the integrand has a branch point $t = 1$, both the Chebyshev and QUADPACK schemes need several hundreds of points compared to TANH and IMT schemes which need at most 128 points. Finally, even though the asymptotic error estimates for TANH and IMT schemes are nearly the same [12], the results of these test problems show that the IMT scheme is clearly superior to the TANH scheme in all the test problems.

5. CONCLUSION

In conclusion, we observe that the accuracy and the efficiency of the IMT scheme which is a modified trapezoidal scheme as adopted by us for the evaluation of CPV integrals are comparable and sometimes superior to those of conventional schemes such as Gauss or Chebyshev. It is particularly suited to integrands having singularities at its end points. Moreover, it performs well even when the integrand has poles close to the line of integration. Last, the generation of nodes and weights is relatively easy.

REFERENCES

1. F. D. Gakhov, *Boundary Value Problems* (Pergamon, Oxford, 1966).
2. R. Piessens, *BIT* **10,** 476 (1970).
3. D. B. Hunter, *Numer. Math.* **19,** 419 (1972).
4. D. F. Paget and D. Elliott, *Numer. Math.* **19,** 373 (1972).
5. M. M. Chawla and N. Jayarajan, *Computing* **15,** 347 (1975).
6. M. Branders and R. Piessens, *J. Comput. Appl. Math.* **1,** 55 (1975).
7. T. Hasegawa and T. Torii, *Math. Comput.* **56,** 741 (1991).
8. J. McNamee, *Math. Comput.* **18,** 368 (1964).
9. C. Schwartz, *J. Comput. Phys.* **4,** 19 (1969).
10. F. Stenger, *J. Inst. Math. Appl.* **12,** 103 (1973).
11. M. Iri, S. Moriguti, and Y. Takasawa, *J. Comput. Appl. Math.* **17,** 3 (1987).
12. H. Takahasi and M. Mori, *Numer. Math.* **21,** 206 (1973).
13. G. Tsamasphyros and P. Androlidakis, *Int. J. Numer. Methods Eng.* **24,** 543 (1987).
14. F. Stenger, *SIAM Rev.* **23,** 165 (1981).
15. B. Bialecki and F. Stenger, *Math. Comput.* **51,** 133 (1988).
16. B. Bialecki, *Math. Comput.* **55,** 665 (1990).
17. B. Bialecki, *BIT* **29,** 464 (1989).