ZASTOSOWANIA MATEMATYKI
APPLICATIONES MATHEMATICAE
20,4 (1990), pp. 591–596

H. V. SMITH (Leeds)

THE NUMERICAL COMPUTATION OF A CLASS OF DIVERGENT INTEGRALS

Abstract. The object of this paper is to present a method of evaluating a class of divergent integrals by replacing part of the integrand by a truncated series of shifted Chebyshev polynomials, the resulting integral then being computed exactly.

1. Introduction. As is well-known, a variety of problems in theoretical physics lead to divergent integrals. In this paper we shall present a method for the numerical computation of a class of divergent integrals of the form

$$I(a) = \int_0^1 t^a f(t)\,dt \tag{1}$$

in which $a < -1$ and $2a$ is non-integral and where the function f is assumed to be regular in some region containing the interval (0, 1).

First, however, let us assume that $f(t) = 1$ and that

$$L(a) = \int_0^1 t^a\,dt. \tag{2}$$

For $a > -1$

$$L(a) = 1/(a+1),$$

but for $a < -1$ and non-integral, expression (2) has no meaning since the integral diverges. Using generalised function theory however, this integral is interpreted as (see [4])

$$L(a) = \int_{-\infty}^{\infty} t^a \big(H(t)-H(t-1)\big)\,dt = 1/(a+1), \qquad a < -1, \tag{3}$$

where

(i) $H(t)$ denotes the Heaviside Unit function defined by

$$H(t) = \begin{cases} 0, & t < 0, \\ 1, & t > 0, \end{cases}$$

(ii) the generalised function $t^a H(t)$ is defined by

$$t^a H(t) = \frac{1}{(a+1)\dots(a+p)}\frac{d^p}{dt^p}(t^{a+p}H(t)),$$

where p is any integer such that $a+p > -1$.

If we now assume $f(t) = T_n^*(t)$, where $T_n^*(t)$ denotes the shifted Chebyshev polynomial of degree n in t, then expression (3) may be used to evaluate integrals of the form

$$M_n(a) = \int_0^1 t^a T_n^*(t)dt \tag{4}$$

for $a < -1$. Indeed, as one may expect, for $a < -1$ and non-integral, generalised function theory interprets this integral as

$$M_n(a) = \int_{-\infty}^{\infty} t^a T_n^*(t)\big(H(t)-H(t-1)\big)dt$$

from which it is easy to deduce (see [4], pp. 31 and 32)

$$M_n(a) = \frac{T_n^*(1)}{(a+1)} - \frac{T_n^{*\prime}(1)}{(a+1)(a+2)} + \dots + \frac{(-1)^n T_n^{*(n)}(1)}{(a+1)\dots(a+n+1)}. \tag{5}$$

This is the Hadamard finite part of the integral in (4) and is what one would formally obtain from (4) by repeated integration by parts if all the contributions from the lower limit (which are infinite) were omitted.

As we have already pointed out, in this paper we shall present a method for the numerical approximation of integrals of the form (1) where the function f is assumed to be regular in some region containing the interval (0, 1).

To begin, the function f in (1) may be approximated by a finite sum of shifted Chebyshev polynomials

$$f(t) \simeq \sum_{n=0}^{N}{}'' a_n T_n^*(t), \quad 0 \leqslant t \leqslant 1, \tag{6}$$

where the double prime indicates that the first and last terms in the sum are to be halved.

It is well-known that the coefficients in (6) are given by (see [2])

$$a_r = \frac{2}{N}\sum_{s=0}^{N}{}'' F_s \cos(\pi rs/N), \tag{7}$$

where

$$F_s = f\big((\cos(\pi s/N)+1)/2\big).$$

Several efficient algorithms are available for their computation ([1], [3]). By substituting (6) into (1) it follows that

$$I(a) \simeq \sum_{n=0}^{N}{}'' a_n M_n(a). \tag{8}$$

2. The numerical evaluation of $M_n(a)$. The shifted Chebyshev polynomial $T_n^*(t)$ satisfies the differential equation (see [6])

$$2t(1-t)y''-(2t-1)y'+2n^2y = 0. \tag{9}$$

Differentiating (9) p times and letting $t = 1$ we see that

$$T_n^{*(p+1)}(1) = \frac{2(n^2-p^2)}{(2p+1)} T_n^{*(p)}(1), \quad 0 \leqslant p \leqslant n-1.$$

If the general term in (5) is denoted by u_j, that is

$$u_j = \frac{(-1)^j T_n^{*(j)}(1)}{(a+1)\dots(a+j+1)},$$

then

$$u_{j+1} = \frac{-2}{(a+j+2)}\left(\frac{n^2-j^2}{2j+1}\right)u_j, \quad 0 \leqslant j \leqslant n-1, \tag{10}$$

and hence

$$M_n(a) = \sum_{j=0}^{n} u_j. \tag{11}$$

Expression (10), starting with $u_0 = 1/(a+1)$, and (11) may now be used to evaluate the $M_n(a)$'s. Incidentally, it is not difficult to see that this method will be sensitive to rounding errors.

Finally, numerical experiments suggest the absolute value of $M_n(a)$ increases as $n \to \infty$, and so we turn our attention to the asymptotic behaviour of a general term of (8). In fact, several authors have already derived the asymptotic behaviour of the coefficients a_n as $n \to \infty$ under the assumption the function f has certain properties, for example regularity within a specified domain (for a summary see [5]), and therefore we only derive the asymptotic behaviour of $M_n(a)$ as $n \to \infty$.

3. Asymptotic behaviour of $M_n(a)$ as $n \to \infty$, a fixed.

THEOREM 1. *For any fixed number $a < -1$ and such that $2a$ is non-integral we have*

$$M_n(a) \sim (-1)^n \mathrm{const}/n^{2a+2} \quad \text{as } n \to \infty.$$

Proof. By making the substitution $t = \cos^2(x\pi/2)$ in (4) it follows that

$$M_n(a) = \pi R \int_0^1 k(x) e^{-2yx\pi i} dx, \tag{12}$$

where

$$k(x) = \cos^{2a+1}(x\pi/2)\sin(x\pi/2), \quad y = n/2.$$

Following Lighthill's prescription [4] the asymptotic behaviour of the integral in (12) may be derived from the behaviour of the Fourier Transform (F.T.)

$$(13)\qquad M_n(a) = \int_{-\infty}^{\infty} k(x)e^{-2yx\pi i}H(x)H(1-x)dx = \int_{-\infty}^{\infty} z(x)e^{-2yx\pi i}dx,$$

where $z(x) = k(x)H(x)H(1-x)$ coincides with $k(x)$ in the interval (0, 1) and is zero elsewhere.

The behaviour of the F.T. in (13) depends critically on the behaviour of $z(x)$ in the neighbourhood of its singularity at $x = 1$ (and not on its behaviour in the neighbourhood of $x = 0$ as applying the present analysis at the point $x = 0$ shows). Indeed if, corresponding to the singularity at $x = 1$, a function $J(x)$ can be constructed that is a linear combination of functions of the types

$$|x-1|^\gamma, \quad |x-1|^\gamma \operatorname{sgn}(x-1), \quad |x-1|^\gamma \ln|x-1|, \quad |x-1|^\gamma \ln|x-1| \operatorname{sgn}(x-1)$$

for different γ and is such that $z(x)-J(x)$ has an absolutely integrable p-th derivative in a neighbourhood of $x = 1$ and which also has as its F.T.

$$(14)\qquad m_n = \int_{-\infty}^{\infty} J(x)e^{-2yx\pi i}dx,$$

then Lighthill showed that an asymptotic expansion for $M_n(a)$ is

$$(15)\qquad M_n(a) = m_n + O(n^{-p})$$

as $n \to \infty$.

In order to apply Lighthill's result we define a function $h(x)$ (which is continuous and has continuous derivatives at $x = 1$) by

$$k(x) = (1-x)^{2a+1}h(x).$$

The construction of $J(x)$ is now obtained from the Taylor expansion of $h(x)$ about the point $x = 1$, that is

$$(16)\qquad J(x) = \sum_{s=0}^{p+[2|a|]-2} \frac{(-1)^s h^{(s)}(1)(1-x)^{2a+s+1}H(1-x)}{s!}.$$

Lighthill ([4], p. 43) actually lists the F.T. that we shall require, namely

$$(17)\qquad \int_{-\infty}^{\infty} (1-x)^{b+s}H(1-x)e^{-2yx\pi i}dx = \frac{e^{i(b+s+1-4y)\pi/2}(b+s)!}{(2\pi|y|)^{b+s+1}},$$

where $b+s$ is non-integral.

From (14)–(17) for $a < -1$ and such that $2a$ is non-integral it follows that

$$\frac{M_n(a)}{\pi} \sim \sum_{s=0}^{p+[2|a|]-2} \frac{(-1)^{s+n}h^{(s)}(1)\cos\big((2a+s+2)\pi/2\big)(2a+s+1)!}{s!(\pi n)^{2a+s+2}} + O(n^{-p}),$$

that is

$$M_n(a) \sim (-1)^n \mathrm{const}/n^{2a+2},$$

as required.

4. Numerical example. The computation of the following example was performed on the Prime 9955 computer at Leeds Polytechnic using double precision except for the computation of the moments which, because of the sensitivity of (10) and (11) to rounding errors, was performed in quadruple precision:

$$\int_0^1 t^{-2.25}/(1+t)dt = 4.174990989.$$

From Theorem 1 with $a = -2.25$ and [6], p. 50, line 4.7–7, it follows that, for the function $f(t) = 1/(1+t)$,

$$|a_n M_n(-2.25)| \sim \mathrm{const}(3-2\sqrt{2})^n n^{2.5} \to 0 \quad \text{as } n \to \infty.$$

In this example our method requires twenty terms of (8) to give the value of the integral correct to 9 decimal places (see Table 1), the Chebyshev coefficients having been approximated by using (7) with $N = 19$ and the moments by using (10) and (11).

Acknowledgement. The author wishes to express his gratitude to the referee for his extremely useful comments and suggestions.

TABLE 1

k	$a_k M_k$
0	−1.1313708499
1	1.7470129473
2	1.7429327930
3	0.8350807383
4	0.2950893294
5	0.0886153356
6	0.0240047777
7	0.0060586537
8	0.0014519784
9	0.0003345069
10	0.0000747006
11	0.0000162674
12	0.0000034693
13	0.0000007272
14	0.0000001503
15	0.0000000306
16	0.0000000057
17	0.0000000019
18	0.0000000002
19	0.0000000001

References

[1] M. Branders and R. Piessens, *Algorithm 001, An extension of Clenshaw–Curtis quadrature*, J. Comput. Appl. Math. (1975), pp. 255–260.

[2] C. W. Clenshaw and A. R. Curtis, *A method for numerical integration on an automatic computer*, Numer. Math. 2 (1960), pp. 197–205.

[3] W. M. Gentleman, *Algorithm 424, Clenshaw–Curtis quadrature*, Comm. ACM 15 (1972), pp. 353–355.

[4] M. J. Lighthill, *An Introduction to Fourier Analysis and Generalised Functions*, Cambridge Monographs Mech. Appl. Math., Cambridge University Press, 1980.

[5] H. O'Hara and F. J. Smith, *Error estimation in the Clenshaw–Curtis quadrature formula*, Comput. J. 11 (1968), pp. 213–219.

[6] M. A. Snyder, *Chebyshev Methods in Numerical Approximation*, Prentice-Hall, Inc., 1966.

HARRY V. SMITH
DEPT. OF INFORMATION SYSTEMS
THE POLYTECHNIC
LEEDS, YORKSHIRE LS6 3QS, ENGLAND

Received on 1988.02.25