Comp. & Maths. with Appls. Vol. 12B, No. 5/6, pp. 1241–1248, 1986
Printed in Great Britain.
0886-9561/86 $3.00 + 0.00

COMPUTATION OF FOURIER AND LAPLACE TRANSFORMS OF SINGULAR FUNCTIONS USING MODIFIED MOMENTS

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(*Received* 16 *January* 1985)

Abstract—In this paper a recurrence formula for the computation of

$$M_k = \int_{-1}^{+1} (1-x)^\alpha (1+x)^\beta \exp[-a/(1+x)] T_k(x)\,dx$$

is presented. The numerical stability is discussed. The starting values are confluent hypergeometric functions which can be evaluated using Luke's results on Chebyshev series expansions and Padé approximations of hypergeometric functions. Applications of this recurrence relation are the evaluation of the Fourier transform of singular functions by modified Clenshaw–Curtis integration, the construction of Gaussian quadrature formulae for Fourier integrals and the numerical inversion of the Laplace transform.

1. INTRODUCTION

Integrals of the form

$$I(p) = \int_0^\infty e^{-pt} f(t)\,dt, \tag{1}$$

where p is a complex parameter, occur frequently in applied mathematics, as Laplace or Fourier transforms. These integrals are difficult to evaluate numerically because of the infinite interval of integration and, when p is not real, because of the oscillatory behaviour of the integrand.

A well-known integration rule for equation (1) is the Gauss–Laguerre formula, but it has good effect only when p is real and $f(t)$ can be approximated accurately by a polynomial. A very interesting survey of more sophisticated integration methods for Fourier and Laplace transform integrals is given by Davis and Rabinowitz [1].

A new method [2] based on Chebyshev polynomial approximations of $f(t)$ is very efficient if $f(t)$ is smooth on $[0, \infty)$ and if there are real numbers $b \neq 0$ and γ such that

$$f(t) \sim b(1+t)^\gamma, \quad t \to \infty. \tag{2}$$

This method, however, is not effective for integrals with singular integrand. The purpose of this paper is to give an extension of it, which is suitable when $f(t)$ has an algebraic singularity at $t = 0$, i.e.

$$f(t) = t^\alpha g(t), \tag{3}$$

where $g(t)$ is smooth on $[0, \infty)$, and $\alpha > -1$. Taking into account expressions (2) and (3), we can write

$$f(t) = t^\alpha (1+t)^{\gamma-\alpha} h(t), \tag{4}$$

where $h(t)$ is a smooth function having a finite and nonzero limit for $t \to 0$ and $t \to \infty$. We consider now the integral

$$I(p) = \int_0^\infty e^{-pt} t^\alpha (1+t)^{\gamma-\alpha} h(t)\,dt. \tag{5}$$

We make the change of variable $t=(1-x)/(1+x)$ in equation (5) yielding

$$I(p)=2^{-\alpha-\beta-1}\exp(a/2)\int_{-1}^{+1}(1-x)^{\alpha}(1+x)^{\beta}\exp[-a/(x+1)]\phi(x)\,\mathrm{d}x, \tag{6}$$

where

$$\beta=-\gamma-2,$$
$$a=2p$$

and

$$\phi(x)=h[(1-x)/(1+x)].$$

Consider now the Chebyshev series approximation

$$\phi(x)\simeq\sum_{k=0}^{N}{}' c_k T_k(x), \tag{7}$$

where the prime denotes summation with the first term halved. Expansion (7) is equivalent to

$$f(t)\simeq t^{\alpha}(1+t)^{-\alpha-\beta-2}\sum_{k=0}^{N}{}' c_k T_k\left(\frac{1-t}{1+t}\right). \tag{8}$$

Substituting expansion (7) into equation (6) yields

$$I(p)\simeq 2^{-\alpha-\beta-1}\exp(a/2)\sum_{k=0}^{N}{}' c_k M_k(\alpha,\beta), \tag{9}$$

where

$$M_k(\alpha,\beta)=\int_{-1}^{+1}(1-x)^{\alpha}(1+x)^{\beta}\exp[-a/(x+1)]T_k(x)\,\mathrm{d}x. \tag{10}$$

For the computation of the coefficients c_k in expansion (7), efficient algorithms based on the FFT are available [3, 4]. The integrals $M_k(\alpha,\beta)$ are modified moments of the weight function $(1-x)^{\alpha}(1+x)^{\beta}\exp[-a/(1+x)]$ [5].

The idea of applying Chebyshev series approximations to the numerical computation of integrals is due to Clenshaw and Curtis [6]. Therefore, computation of $I(p)$ using formula (9) is termed "modified Clenshaw–Curtis quadrature" (MCC-quadrature).

A recurrence relation for the computation of $M_k(\alpha,\beta)$, $k=0,1,2,\ldots$, is given in Section 2. The numerical aspects of this recurrence relation and the computation of the starting values are considered in Sections 3 and 4.

Apart from their application in MCC-quadrature, modified moments figure also in other domains of numerical integration, such as in constructing Gaussian quadrature formulae [7, 5]. This application is considered in Section 5.

The Bromwich integral for the inversion of Laplace transforms [8] can be transformed into an integral of form (1), with purely imaginary p. This means that the MCC-quadrature developed in this paper can be useful for numerical Laplace transform inversion. This is the subject of Section 6.

2. A RECURRENCE RELATION FOR $M_k(\alpha,\beta)$

The sequence $M_k(\alpha,\beta)$, $k=0,1,2,\ldots$, satisfies the following linear, homogeneous, five-term recurrence relation [instead of $M_k(\alpha,\beta)$ we write M_k]:

$$(\alpha+\beta+3+k)M_{k+2}+2(a+2\alpha+2+k)M_{k+1}+2(3\alpha-\beta-2a+1)M_k$$
$$+2(a+2\alpha+2-k)M_{k-1}+(\alpha+\beta+3-k)M_{k-2}=0. \tag{11}$$

Proof

Let

$$J = \int_{-1}^{+1} (1-x)^{\alpha+1}(1+x)^{\beta+2}\exp[-a/(1+x)]\,T_k'(x)\,\mathrm{d}x. \tag{12}$$

Using the identity

$$(1-x^2)T_k'(x) = k[T_{k-1}(x) - T_{k+1}(x)]/2$$

equation (12) can be written in the form

$$J = k(M_{k-2} + 2M_{k-1} - 2M_{k+1} - M_{k+2})/4. \tag{13}$$

On the other hand, integration by parts of equation (12) yields

$$J = (\alpha+1)M_k(\alpha, \beta+2) - (\beta+2)M_k(\alpha+1, \beta+1) - aM_k(\alpha+1, \beta). \tag{14}$$

Now, since $2xT_k(x) = T_{k+1}(x) + T_{k-1}(x)$, we have

$$M_k(\alpha+1, \beta) = M_k - (M_{k+1} + M_{k-1})/2,$$

$$M_k(\alpha+1, \beta+1) = M_k/2 - (M_{k+2} + M_{k-2})/4$$

and

$$M_k(\alpha, \beta+2) = 3M_k/2 + M_{k+1} + M_{k-1} + (M_{k+2} + M_{k-2})/4.$$

Equating equations (13) and (14) yields relation (11). ■

3. NUMERICAL STABILITY OF THE RECURRENCE RELATION

The numerical stability of forward recursion, backward recursion or any other algorithm for solving relation (11) depends on the asymptotic behaviour of M_k with respect to the asymptotic behaviour of all other solutions of relation (11), for $k \to \infty$.

Recurrence relation (11) is a Poincaré difference equation with the pseudo-characteristic equation

$$\lambda^4 + 2\lambda^3 - 2\lambda - 1 = 0$$

which has a simple root $\lambda_1 = 1$ and a triple root $\lambda_2 = -1$.

The asymptotic behaviour of four independent solutions $y_{i,k}$, $i = 1, 2, 3, 4$, $k \to \infty$, is given by [9, 10]:

$$y_{1,k} \sim k^{-2(\alpha+1)}$$

and

$$y_{i,k} \sim (-1)^k \exp(\gamma_i k^{2/3}) k^{-1-2\beta/3}, \quad i = 2, 3, 4,$$

where

$$\gamma_2 = 3(a/2)^{1/3},$$

$$\gamma_3 = 3(-1/2 + j\sqrt{3}/2)(a/2)^{1/3}$$

and

$$\gamma_4 = -3(1/2 + j\sqrt{3}/2)(a/2)^{1/3}.$$

If a is real and positive, then, for large values of k, $|y_{2,k}|$ is an exponentially increasing sequence and $|y_{1,k}|$, $|y_{3,k}|$ and $|y_{4,k}|$ are decreasing.

If $a = -j\omega$, then

$$\gamma_2 = 3j\omega^{1/3},$$

$$\gamma_3 = -3(\sqrt{3} + j)\omega^{1/3}/2$$

and

$$\gamma_4 = 3(\sqrt{3} - j)\omega^{1/3}/2.$$

In this case $|I_k^{(4)}|$ is strongly increasing.

The sequence M_k shows the asymptotic behaviour

$$M_k(\alpha, \beta) = O(k^{-2(\alpha+1)}), \quad k \to \infty.$$

Comparing M_k and $y_{i,k}$, we can conclude that forward and backward recursion of relation (11) are numerically unstable, but that for reasonable values of α and β, Oliver's algorithm [11] or Lozier's algorithm [12] with three starting values $M_0(\alpha, \beta)$, $M_1(\alpha, \beta)$ and $M_2(\alpha, \beta)$ are stable.

4. COMPUTATION OF THE STARTING VALUES M_0, M_1 AND M_2

Comparing the integral expression of the Whittaker function $W_{\mu,\nu}(z)$ (see Luke [13, p. 212]), with

$$M_0(\alpha, \beta) = 2^{\alpha+\beta+1} \exp(-a/2) \int_0^\infty u^\alpha (1+u)^{-\alpha-\beta-2} \exp(-au/2) \mathrm{d}u, \tag{15}$$

yields

$$M_0(\alpha, \beta) = 2^{\alpha+1}(2a)^{\beta/2} \exp(-a/4) \Gamma(\alpha+1) W_{-\alpha-1-\beta/2, (\beta+1)/2}(a/2). \tag{16}$$

Using the relation between Whittaker's function and Kummer's confluent hypergeometric function (see Luke [14, p. 295]), $M_0(\alpha, \beta)$ can also be expressed as

$$M_0(\alpha, \beta) = 2^\alpha \exp(-a/2) \Gamma(\alpha+1) a^{\beta+1} U(\alpha+\beta+2, \beta+2, a/2) \tag{17}$$

or

$$M_0(\alpha, \beta) = 2^{\alpha+\beta+1} \exp(-a/2) \Gamma(\alpha+1) U(\alpha+1, -\beta, a/2), \tag{18}$$

where

$$U(p, q, z) = \frac{\pi}{\sin q\pi} \left| \frac{{}_1F_1(p, q, z)}{\Gamma(1+p-q)\Gamma(q)} - z^{1-q} \frac{{}_1F_1(1+p-q, 2-q, z)}{\Gamma(p)\Gamma(2-q)} \right|. \tag{19}$$

The computation of the confluent hypergeometric functions ${}_1F_1(p, q, z)$ and $U(p, q, z)$ are discussed in detail by Luke [14, p. 284; 15, p. 88].

For small values of $|z|$, the power series expansion or expansions in series of Chebyshev polynomials or Bessel functions can be used.

For large $|z|$, the asymptotic expansion

$$U(p, q, z) \sim z^{-p} {}_2F_0(p, 1+p-q; -z^{-1}) \tag{20}$$

is useful. The remainder for this asymptotic formula is discussed by Luke [16, p. 127].

If $\alpha = 0$, then

$$M_0(0, \beta) = a^{\beta+1} \Gamma(-\beta-1, a/2), \tag{21}$$

where

$$\Gamma(\nu, z) = \int_z^\infty e^{-t} t^{\nu-1} \mathrm{d}t$$

is the incomplete Γ function.

Padé approximations for $\Gamma(\nu, z)$ are provided by Luke [17, p. 186]. The other starting values can be computed using

$$M_1(\alpha, \beta) = M_0(\alpha, \beta+1) - M_0(\alpha, \beta) = -M_0(\alpha+1, \beta) + M_0(\alpha, \beta) \tag{22}$$

and

$$M_2(\alpha, \beta) = [(\beta + 2a - 3\alpha - 1) M_0(\alpha, \beta) - 2(2\alpha + a + 2) M_1(\alpha, \beta)]/(\alpha + \beta + 3). \tag{23}$$

5. MODIFIED MOMENTS FOR THE CONSTRUCTION OF GAUSSIAN QUADRATURE FORMULAE

Krylov and Kruglikova [18] have published abscissae x_k and weights w_k of the quadrature formulae

$$\int_0^\infty w(t)f(t)\,\mathrm{d}t \simeq \sum_{k=1}^{N} w_k f(t_k), \tag{24}$$

where $w(t) = 1 + \sin t$ or $w(t) = 1 + \cos t$, which are of maximal degree of precision, i.e. they are exact for $2N$ linearly independent functions $(t+1)^{\gamma-l}$, $l = 0, 1, \ldots, 2N-1$, where $\gamma < -1$ is a real parameter. The main application of these formulae is the numerical evaluation of Fourier integrals.

The abscissae t_k are the zeros of a polynomial

$$\omega_N(t) = \sum_{i=0}^{N} a_i(1+t)^i. \tag{25}$$

The coefficients a_i of $\omega_N(t)$ are the solution of the system of linear equations

$$\sum_{i=0}^{N} a_i \int_0^\infty w(t)(1+t)^{\gamma-2N+1+i+j}\,\mathrm{d}t = 0, \tag{26}$$

where $a_N = 1$, and $j = 0, 1, \ldots, N-1$.

Unfortunately, system (26) is not well-conditioned. Consequently, it is not possible to construct quadrature formulae of high or even moderate degree, using this method.

Gautschi [5] has shown that constructing Gaussian quadrature formulae can be well-conditioned if modified moments are used. He has given also an algorithm for solving this problem. The modified moments required for computing w_k and t_k in formula (24) are

$$\int_0^\infty (1+t)^\gamma\{1 + \mathscr{R}e[\exp(jt)]\}\, T_k^*\left(\frac{1}{1+t}\right)\mathrm{d}t$$

if $w(t) = 1 + \cos t$ and

$$\int_0^\infty (1+t)^\gamma\{1 + \mathscr{I}m[\exp(jt)]\}\, T_k^*\left(\frac{1}{1+t}\right)\mathrm{d}t$$

if $w(t) = 1 + \sin t$, for $k = 0, 1, \ldots, 2N-1$, which are closely related to $[M_k(0, -\gamma-2)]_{a=-2j}$.

In Table 1 we present the abscissae and weights of equation (24) for $w(t) = 1 + \cos t$, $N = 20$ and $\gamma = -2$. In Table 2, the corresponding formula for $w(t) = 1 + \sin t$ is given.

Table 1. Quadrature formula for

$$\int_0^\infty (1+\cos t)f(t)\mathrm{d}t \simeq \sum_{k=1}^{20} w_k f(t_k) \quad (\gamma = -2)$$

	Abscissae	Weights
1	0.3386058170 (−2)	0.1741771523 (−1)
2	0.1801020822 (−1)	0.4131393391 (−1)
3	0.4502727059 (−1)	0.6714079441 (−1)
4	0.8572392573 (−1)	0.9609997883 (−1)
5	0.1421157751 (0)	0.1296097617 (0)
6	0.2171622912 (0)	0.1693026298 (0)
7	0.3150977485 (0)	0.2169337099 (0)
8	0.4419437824 (0)	0.2739782108 (0)
9	0.6063087818 (0)	0.3404359468 (0)
10	0.8206586880 (0)	0.4117568620 (0)
11	0.1103418203 (1)	0.4718025908 (0)
12	0.1482820350 (1)	0.4797930605 (0)
13	0.2007027532 (1)	0.3606207757 (0)
14	0.2993995123 (1)	0.1267414533 (0)
15	0.4826393636 (1)	0.1772377054 (1)
16	0.6672548233 (1)	0.4110397414 (1)
17	0.1208492846 (2)	0.6660843999 (1)
18	0.2249622365 (2)	0.1640498468 (2)
19	0.5569738285 (2)	0.6359863965 (2)
20	0.2953289385 (3)	0.7591174214 (3)

Table 2. Quadrature formula for

$$\int_0^\infty (1+\sin t)f(t)\,dt \simeq \sum_{k=1}^{20} w_k f(t_k) \quad (\gamma = -2)$$

	Abscissae	Weights
1	0.3501154308 (−2)	0.9037089350 (−2)
2	0.1862818942 (−1)	0.2177380870 (−1)
3	0.4659867371 (−1)	0.3641277897 (−1)
4	0.8878961532 (−1)	0.5437519462 (−1)
5	0.1473629100 (0)	0.7766888483 (−1)
6	0.2255013491 (0)	0.1092721767 (0)
7	0.3277727148 (0)	0.1537548375 (0)
8	0.4606933302 (0)	0.2182242402 (0)
9	0.6336028158 (0)	0.3135932151 (0)
10	0.8600346245 (0)	0.4555509858 (0)
11	0.1159892182 (1)	0.6621211650 (0)
12	0.1562980918 (1)	0.9363687734 (0)
13	0.2115135094 (1)	0.1202587676 (1)
14	0.2892727915 (1)	0.1162294213 (1)
15	0.4249267867 (1)	0.4708812811 (0)
16	0.7225521283 (1)	0.4443383411 (1)
17	0.1172452441 (2)	0.5759050538 (1)
18	0.2173967597 (2)	0.1615603009 (2)
19	0.5433333584 (2)	0.6234293067 (2)
20	0.2890827091 (3)	0.7435723979 (3)

Numerical example

We evaluate

$$I(\omega) = \int_0^\infty \frac{t \sin \omega t}{\sqrt{(t^2+1)^3}}\,dt. \tag{27}$$

The exact value is

$$I(\omega) = \omega K_0(\omega),$$

where $K_0(\omega)$ is the modified Bessel function of the second kind.

We write

$$I(\omega) = \omega \int_0^\infty \frac{u(1+\sin u)}{\sqrt{(u^2+\omega^2)^3}}\,du - 1. \tag{28}$$

The integral in equation (28) is evaluated using the 10-point (see Krylov and Kruglikova [18, p. 100]) and 20-point (see Table 2) quadrature formulae. The absolute errors are reported in Table 3.

6. LAPLACE TRANSFORM INVERSION

Let $F(p)$ be the Laplace transform of $f(t)$. In many applications, it is necessary to find $f(t)$, given the Laplace transform $F(p)$. It is well-known that the solution of this problem

Table 3. Numerical integration of

$$\int_0^\infty \frac{t \sin at}{\sqrt{(t^2+1)^3}}\,dt$$

a	Exact integral	Absolute error ($N = 10$)	Absolute error ($N = 20$)
1.0	0.421024438241	−0.15 (−6)	−0.13 (−12)
2.0	0.227787745499	0.54 (−6)	−0.24 (−12)
3.0	0.104218513159	0.47 (−5)	0.46 (−11)
4.0	0.044638704344	−0.10 (−4)	0.77 (−10)
5.0	0.018455491670	−0.61 (−4)	−0.80 (−9)
6.0	0.007463965968	0.67 (−4)	0.34 (−8)
7.0	0.002973570193	0.36 (−3)	0.66 (−8)
8.0	0.001171765642	0.54 (−3)	−0.57 (−7)
9.0	0.000457931817	0.33 (−3)	−0.10 (−6)
10.0	0.000177800623	−0.38 (−3)	0.16 (−6)

is given by the Bromwich integral [8]

$$f(t) = \frac{1}{2\pi j} \int_{c-j\infty}^{c+j\infty} e^{pt} F(p)\,dp, \tag{29}$$

where c is a real number such that $F(p)$ is an analytic function for $\mathscr{Re}(p) > c$.

Making the substitution $p = c + j\omega$, we obtain

$$f(t) = \frac{2}{\pi} \exp(ct) \int_0^\infty \cos \omega t \quad \phi(\omega)\,d\omega, \tag{30}$$

where

$$\phi(\omega) = \mathscr{Re}[F(c + j\omega)].$$

The integral (30) can be computed using the MCC-method, described above. The following numerical examples show that this method of numerical inversion is competitive with the best methods considered in the comparative study of Davies and Martin [19].

Example 1

$$F(p) = \frac{1}{\sqrt{1 + p^2}}$$

and

$$f(t) = J_0(t).$$

Since $F(p)$ has branchpoints at $p = \pm j$, c has to be positive. Since

$$\phi(\omega) = \mathscr{Re}\left(\frac{1}{\sqrt{1 + (c + j\omega)^2}}\right) \sim \frac{c}{\omega^2}, \quad \omega \to \infty,$$

we apply the MCC-method with $\alpha = 0$ and $\gamma = -2$ or $\beta = 0$.

In Table 4 we give results for $c = 1$, $N = 96$ and $c = 2$, $N = 48$.

Table 4. Numerical inversion of $\dfrac{1}{\sqrt{1+p^2}}$

t	Exact	Relative error $c = 1, N = 96$	Relative error $c = 2, N = 48$
1.00	0.76519768655797	−0.63(−15)	−0.19(−14)
2.00	0.22389077914124	0.18(−13)	−0.23(−11)
3.00	−0.26005195490193	0.11(−15)	0.57(−10)
4.00	−0.39714980986385	−0.56(−13)	−0.52(−9)
5.00	−0.17759677131434	−0.16(−11)	−0.55(−8)
6.00	0.15064525725100	−0.64(−11)	−0.98(−7)
7.00	0.30007927051956	0.51(−11)	0.40(−6)
8.00	0.17165080713755	−0.78(−11)	−0.47(−5)
9.00	−0.09033361118288	−0.14(−8)	−0.54(−4)
10.00	−0.24593576445135	0.60(−9)	−0.38(−4)
20.00	0.16702466434058	0.25(−3)	0.30(6)

Example 2

$$F(p) = \log \frac{p + 2}{p + 1}$$

and

$$f(t) = (e^{-t} - e^{-2t})/t.$$

Since $F(p)$ has a singularity at $p = -1$, we have to choose $c > -1$. Since

$$\phi(\omega) = \mathscr{Re}\left(\log \frac{c + 2 + j\omega}{c + 1 + j\omega}\right) \sim \frac{c + 3/2}{\omega^2}, \quad \omega \to \infty,$$

we apply the MCC-method with $\alpha = 0$ and $\gamma = -2$ or $\beta = 0$.

Table 5. Numerical inversion of $\log[(p+1)/(p+2)]$

t	Exact	Relative error $c=-0.95, N=96$	Relative error $c=-0.5, N=24$
1.00	0.23254415793483 (0)	−0.38 (−14)	0.52 (−11)
2.00	0.58509822173939 (−1)	0.34 (−13)	−0.10 (−10)
3.00	0.15769438730399 (−1)	0.51 (−12)	0.41 (−10)
4.00	0.44950440652079 (−2)	−0.19 (−12)	−0.10 (−9)
5.00	0.13385094138646 (−2)	−0.85 (−12)	−0.61 (−12)
6.00	0.41210132728550 (−3)	−0.91 (−12)	0.90 (−9)
7.00	0.13015006240506 (−3)	0.18 (−12)	−0.10 (−8)
8.00	0.41918761590974 (−4)	0.20 (−11)	−0.47 (−8)
9.00	0.13710508234104 (−4)	−0.10 (−11)	0.19 (−8)
10.00	0.45397868608862 (−5)	−0.72 (−12)	0.22 (−7)
20.00	0.10305768090951 (−9)	−0.44 (−11)	−0.48 (−6)
30.00	0.31192076562798 (−14)	0.89 (−10)	0.18 (−2)
40.00	0.10620885638229 (−18)	−0.20 (−9)	−0.24 (0)
50.00	0.38574996959278 (−23)	0.41 (−9)	0.43 (1)
60.00	0.14594184604494 (−27)	0.12 (−9)	0.45 (4)

In Table 5 we give results for $c=-0.95$, $N=96$ and $c=-0.5$, $N=24$.

Acknowledgement—This research was supported by the "Onderzoeksfonds" of the Catholic University of Leuven.

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