The Evaluation of a Class of Functions Defined by an Integral

By D. B. Hunter

1. In [4] the author described a method of evaluating the modified Bessel function of the second kind, $K_n(z)$, based on approximating by the trapezoidal rule the integral representation

$$(1) \qquad K_n(z) = \frac{\sqrt{\pi}e^{-z}}{\Gamma(n+\frac{1}{2})(2z)^n} \int_{-\infty}^{\infty} e^{-t^2} t^{2n} (2z + t^2)^{n-1/2} dt\,,$$

([4, Eq. (5)]). Here z is a general complex number:

$$(2) \qquad z = x + iy = \rho e^{i\theta}\,.$$

In the present paper we consider a number of other functions which can be evaluated similarly.

We shall express the functions in terms of the integral

$$(3) \qquad G_r(m; n_1, \lambda_1; n_2, \lambda_2; \cdots; n_r, \lambda_r; z) = \int_0^{\infty} 2e^{-t^2} t^{2m} \prod_{j=1}^{r} (\lambda_j z + t^2)^{n_j} dt\,.$$

Here the exponents $m, n_1, n_2, \cdots, n_r$ are real, with $m > -\frac{1}{2}$, and, in the examples we shall consider, the parameters $\lambda_1, \lambda_2, \cdots, \lambda_r$ are real and positive. Under those circumstances the integral (3) will converge provided $\rho > 0$ and $|\theta| < \pi$, the last condition being imposed to avoid possible singularities of the integrand on the positive real axis. In some cases (3) will also converge when $\rho = 0$. In general, for brevity, we shall denote this function by $G_r(m; n, \lambda; z)$.

The following alternative expression is easily derived:

$$(4) \qquad G_r(m; n, \lambda; z) = \rho^{m+n+1/2} \int_0^{\infty} 2e^{-t^2} t^{2m} \prod_{j=1}^{r} (\lambda_j e^{i\theta} + t^2)^{n_j} dt$$

where

$$(5) \qquad n = n_1 + n_2 + \cdots + n_r\,.$$

Again, this expression is valid provided $\rho > 0$ and $|\theta| < \pi$.

2. Examples. Before considering the numerical evaluation of $G_r(m; n, \lambda; z)$, we list a number of special functions which can be expressed in terms of it. Some of the examples are, of course, related.

(i) *The gamma function*, $\Gamma(a)$.

$$(6) \qquad \Gamma(a) = G_0(a - \tfrac{1}{2}; z)\,.$$

This is, of course, independent of z.

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(ii) *The incomplete gamma function,* $\Gamma(a, z) = \int_z^\infty t^{a-1}e^{-t}dt.$

$$\Gamma(a, z) = \frac{e^{-z}z^a}{\Gamma(1-a)} G_1(\tfrac{1}{2} - a; -1, 1; z) \quad \text{if} \quad R(a) < 1\,, \tag{7}$$

(cf. Luke [6, 7.3(3)]).

(iii) *The complementary error function,* $\operatorname{erfc}(z) = (2/\sqrt{\pi}) \int_z^\infty e^{-t^2}dt.$

$$\operatorname{erfc}(z) = (z/\pi)e^{-z^2}G_1(0; -1, 1; z^2)\,, \tag{8}$$

(see Fettis [2, § 4]).

(iv) *Kummer's confluent hypergeometric function,* $U(a, b, z)$.

$$U(a, b, z) = \frac{1}{\Gamma(a)z^{b-1}} G_1(a - \tfrac{1}{2}; b - a - 1, 1; z)\,, \tag{9}$$

(cf. Abramowitz and Stegun [1, 13.2.5]).

(v) *The modified Bessel function,* $K_n(z)$.

$$K_n(z) = \frac{\sqrt{\pi}e^{-z}}{\Gamma(n + \frac{1}{2})(2z)^n} G_1(n; n - \tfrac{1}{2}, 2; z)\,, \tag{10}$$

(see (1)).

(vi) *The integral* $\int_z^\infty e^{-pu}u^m K_n(\lambda u)du$, *(m, n integers, with* $m + n \geqq 0, \lambda + p \geqq 0$*)*, —cf. Luke [6, Chapters IV, V].

$$\begin{aligned}&\int_z^\infty e^{-pu}u^m K_n(\lambda u)du \\ &= \frac{\sqrt{\pi}z^{m-n+1}e^{-(p+\lambda)z}}{(2\lambda)^n\Gamma(n + \frac{1}{2})} \sum_{r=0}^{m+n} \frac{(m+n)!}{r!} G_2(n; n - \tfrac{1}{2}, 2\lambda; r - m - n - 1, \lambda + p; z)\,.\end{aligned} \tag{11}$$

In particular,

$$\int_z^\infty e^{-pu}u^{-n}K_n(u)du = \frac{\sqrt{\pi}z^{1-2n}e^{-(p+\lambda)z}}{(2\lambda)^n\Gamma(n + \frac{1}{2})} G_2(n; n - \tfrac{1}{2}, 2\lambda; -1, \lambda + p; z)\,. \tag{12}$$

A number of special cases of interest arise on giving particular values to the parameters. For example, when $p = 0$, $\lambda = 1$, we have functions similar to some of those considered in Luke [6, Chapter II]. Also, putting $m = n = 0$, $p = 1$, $z = \pm iy$, we obtain integrals of the Schwarz type,—cf. Luke [6, Chapter X]. This example was suggested to the author by the referee.

(vii) *Repeated integrals of* $K_0(z)$. In the notation of Abramowitz and Stegun [1, Chapter 11], let $Ki_0(z) = K_0(z)$, while for $n \geqq 1$

$$Ki_n(z) = \int_z^\infty Ki_{n-1}(u)du\,.$$

Then

$$Ki_n(z) = z^n e^{-z}G_2(0; -n, 1; -\tfrac{1}{2}, 2; z)\,. \tag{13}$$

Similar but more complicated expressions exist for repeated integrals of $e^{-pz}z^m K_n(\lambda z)$.

3. Evaluation of $G_r(m; n, \lambda; z)$. For the remainder of this paper we shall assume that m is a nonnegative integer, so that the integrands in (3) and (4) are even functions of t. In this case it is known (see, e.g., Goodwin [3]) that the integrals can be approximated very closely by the trapezoidal rule, or by Luke's modified form of it, [5]. For simplicity, we shall consider the standard trapezoidal rule.

Suppose $F(w)$ is an even, analytic function of a complex variable w, and that $\int_0^\infty 2F(t)dt$ converges. If we now write the trapezoidal rule with interval h in the form

$$\int_0^\infty 2F(t)dt \equiv \int_{-\infty}^\infty F(t)dt = h\left[F(0) + 2\sum_{r=1}^\infty F(rh)\right] - E(h)\,, \tag{14}$$

it is easy to show, by integrating $F(w)/(1 - e^{-2\pi w/h})$ round a rectangular contour Γ with vertices at $\pm\infty \pm ia$, that

$$E(h) = 2e^{-2\pi a/h}\int_{-\infty}^\infty \frac{e^{-2\pi it/h}F(t - ia)dt}{1 - e^{-2\pi a/h - 2\pi it/h}}\,. \tag{15}$$

The reasoning is similar to that of Goodwin [3]. Here a is any real number such that Γ contains no singularities of $F(w)$. It follows that

$$|E(h)| \leqq \frac{2e^{-2\pi a/h}}{1 - e^{-2\pi a/h}}\int_{-\infty}^\infty |F(t - ia)|dt\,, \tag{16}$$

and this inequality holds also for Luke's modified trapezoidal rule.

We are interested in integrands of the form

$$F(t) = e^{-t^2}t^{2m}\prod_{j=1}^r (\lambda_j z + t^2)^{n_j}$$

or

$$F(t) = e^{-\rho t^2}t^{2m}\prod_{j=1}^r (\lambda_j e^{i\theta} + t^2)^{n_j}\,.$$

For clarity, we shall denote by $E_1(h)$ and $E_2(h)$ respectively the errors in evaluating integrals of those two types by the trapezoidal rule. Thus letting

$$g(a, h, \rho) = 2e^{a(\rho a - 2\pi/h)}/(1 - e^{-2\pi a/h})\,, \tag{17}$$

it follows from (16) that

$$|E_1(h)| \leqq g(a, h, 1)\int_{-\infty}^\infty e^{-t^2}|t - ia|^{2m}\prod_{j=1}^r |\lambda_j z + (t - ia)^2|^{n_j}dt \tag{18}$$

while

$$|E_2(h)| \leqq g(a, h, \rho)\int_{-\infty}^\infty e^{-\rho t^2}|t - ia|^{2m}\prod_{j=1}^r |\lambda_j e^{i\theta} + (t - ia)^2|^{n_j}dt\,. \tag{19}$$

If we denote by μ the smallest of the parameters λ_j for which n_j is not a positive integer, the constant a in (18) and (19) is subject to the restriction

$$\begin{aligned} a &< (\mu\rho)^{1/2}\cos\theta/2 \quad \text{in} \quad (18) \\ &< \mu^{1/2}\cos\theta/2 \quad \text{in} \quad (19)\,. \end{aligned} \tag{20}$$

It remains to obtain upper bounds for the errors. Consider, first, E_1. It is convenient to arrange the factors in the integrand in (3) so that the first p, say, of the exponents n_j are positive, the rest being negative. If we now denote by λ the largest of the parameters $\lambda_1, \lambda_2, \cdots, \lambda_p$, it is easy to show that

$$\prod_{j=1}^{p} |\lambda_j z + (t - ia)^2|^{n_j} \leqq \phi(\nu)\{(\lambda\rho + a^2)^\nu + t^{2\nu}\} \tag{21}$$

where

$$\nu = n_1 + n_2 + \cdots + n_p \tag{22}$$

and

$$\begin{aligned} \phi(\nu) &= 1 \quad \text{if} \quad \nu \leqq 1\,, \\ &= 2^{\nu-1} \quad \text{if} \quad \nu > 1\,. \end{aligned} \tag{23}$$

For $j > p$, we have

$$|\lambda_j z + (t - ia)^2| \geqq (1/\sqrt{2})[|\lambda_j x + t^2 - a^2| + |\lambda_j y - 2at|]\,.$$

Denoting by $\mu_j(a, z)$ the minimum value of the expression on the right as t varies, it can be shown that $\mu_j(a, z)$ is the smallest of the quantities

$$(1/\sqrt{2})\lambda_j(|x| + ||y| - 2a^2|)\,, \qquad (1/\sqrt{2})|\lambda_j x + (\lambda_j y/2a)^2 - a^2|\,,$$

and, if $\lambda_j x \leqq a^2$,

$$(1/\sqrt{2})|\lambda_j|y| - 2a(a^2 - \lambda_j x)^{1/2}|\,.$$

Now, setting

$$\mu(a, z) = \prod_{j=p+1}^{r} [\mu_j(a, z)]^{n_j}\,, \tag{24}$$

we deduce from (18) that

$$|E_1(h)| \leqq g(a, h, 1)\int_{-\infty}^{\infty} \phi(m)\phi(\nu)\mu(a, z)e^{-t^2}(a^{2m} + t^{2m})[(\lambda\rho + a^2)^\nu + t^{2\nu}]dt\,,$$

i.e.,

$$\begin{aligned} |E_1(h)| \leqq\ & g(a, h, 1)\phi(m)\phi(\nu)\mu(a, z) \\ & \times \{a^{2m}(\lambda\rho + a^2)^\nu\Gamma(\tfrac{1}{2}) + (\lambda\rho + a^2)^\nu\Gamma(m + \tfrac{1}{2}) \\ & + a^{2m}\Gamma(\nu + \tfrac{1}{2}) + \Gamma(m + \nu + \tfrac{1}{2})\}\,. \end{aligned} \tag{25}$$

Similarly,

$$\begin{aligned} |E_2(h)| \leqq\ & g(a, h, \rho)\phi(m)\phi(\nu)\mu(a, e^{i\theta}) \\ & \times \{a^{2m}(\lambda + a^2)^\nu\Gamma(\tfrac{1}{2})/\rho^{1/2} + (\lambda + a^2)^\nu\Gamma(m + \tfrac{1}{2})/\rho^{m+1/2} \\ & + a^{2m}\Gamma(\nu + \tfrac{1}{2})/\rho^{\nu+1/2} + \Gamma(m + \nu + \tfrac{1}{2})/\rho^{m+\nu+1/2}\}\,. \end{aligned} \tag{26}$$

A few general comments can be made. Consider, first, $E_1(h)$. The most rapidly-varying factor on the right in (25) is $e^{a(a-2\pi/h)}$, and this has its minimum value,

$\exp[-\pi^2/h^2]$ when $a = \pi/h$. This is therefore a convenient value to use, provided it does not violate the condition (20), that is, provided ρ is not too small. This, in turn, suggests that the method is most suitable for large values of ρ. However, even when ρ is fairly small, good accuracy can often be obtained; for example, it was shown in [4] that $K_0(2)$ can be estimated in this way, using an interval $h = \frac{1}{2}$, with a relative error of order 10^{-9}.

The discussion of $E_2(h)$ is less clear-cut. The factor $e^{a(\rho a - 2\pi/h)}$ in (17) has its minimum value, $\exp[-\pi^2/\rho h^2]$, when $a = \pi/\rho h$. Since this value increases with ρ, progressively smaller values of h must be used as ρ increases in order to maintain accuracy. This disadvantage is largely off-set, however, by the rapid convergence of the integral in (4) for large ρ. If $\rho < 1$, on the other hand, the value $a = \pi/h\rho$ is likely to violate the restriction (20). However, this affects (19) less than (18), and so we expect greater accuracy, for a given value of h, from (4) for small ρ. Unfortunately, as $\rho \to 0$, the rate of convergence of the integral in (4) decreases considerably, and neither form is really suitable for very small values of ρ.

The actual numerical estimation of the error from (18) or (19) is rather tedious, and, since the bounds obtained are, in any case, rather conservative, it may be preferable to establish the error in an actual example by numerical experiment. As an example, we shall estimate the error in calculating $\int_x^\infty t^{-1}K_1(t)dt$ for small, real x, using (4). From (12),

$$\int_x^\infty t^{-1}K_1(t)dt = \frac{e^{-x}}{x} G_2(1; \tfrac{1}{2}, 2; -1, 1; x) .$$

Thus $\lambda = 2$, $\nu = \frac{1}{2}$, $\phi(\nu) = 1$. Also, it can be shown that $\mu(a, 1) = \sqrt{2}/|1 - a^2|$. Thus

$$|E_2(h)| \leqq \frac{2\sqrt{2}e^{a(xa-2\pi/h)}}{(1-a^2)(1-e^{-2\pi a/h})} \left\{ \left(\frac{\pi(a^2+2)}{x} \right)^{1/2} \left(a^2 + \frac{1}{2x} \right) + \frac{1}{x} \left(a^2 + \frac{1}{x} \right) \right\} ,$$

where, from (20), $a < 1$.

If, for example, $h = \frac{1}{4}$, the minimum of the right-hand side occurs near $a = 0.96$, for small x. Using this value, we get, e.g.,

when $x = 1$, $|E_2| \leqq 1.9 \times 10^{-8}$,

when $x = 0.5$, $|E_2| \leqq 2.7 \times 10^{-8}$.

The actual errors for those two values of x were found, by numerical experiment, to be about 2×10^{-10} and 4×10^{-11} respectively.

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