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A double integral containing the modified Bessel function: asymptotics and a device for computation

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A Double Integral Containing the Modified Bessel Function: Asymptotics and a Device for Computation

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A two-dimensional integral containing $exp(-\xi-\eta)I_0(2\sqrt{\xi\eta})$ is considered. $I_0(z)$ is the modified Bessel function and the integral is taken over the rectangle $0 \leqslant \xi \leqslant x$, $0 \leqslant \eta \leqslant y$. The integral is difficult to compute when x and y are large, especially when x and y are almost equal. Computer programs based on existing series expansions are inefficient in this case. A representation in terms of the error function (normal distribution function) is given, from which more efficient and reliable algorithms can be constructed.

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1. Introduction

We consider the Bessel function integral

$$I(x,y) = \int_0^x \int_0^y e^{-\xi-\eta} I_0(2\sqrt{\xi\eta})\, d\xi\, d\eta, \tag{1.1}$$

where $x,y \geqslant 0$ and $I_0(z)$ is the modified Bessel function. Integrals of this type are encountered in many physical contexts; GOLDSTEIN (1953) is a good example. A more recent paper of LASSEY (1982) gives various references on applications. In that paper the computational problem is extensively discussed, not for (1.1) but for related integrals. The algorithms are based on series expansions in terms of modified Bessel functions (see our result (2.7)) or exponential polynomials of the type $\Sigma_{m=0}^{n} x^m / m!$. These expansions are very convenient to implement and they give efficient algorithms in the (x,y) -plane except in the neighborhood of the diagonal. So we don't consider the computational problem completely solved.

When x and y are large and $|x-y|$ is small compared with those two, the integral (1.1) has a peculiar behaviour. To see this, consider the well-known estimate

$$I_0(z) \sim \frac{e^z}{\sqrt{2\pi z}} \text{ as } z \to \infty.$$

It follows that in the far parts of the quarter plane the integrand is exponentially small, except near the diagonal, where we can see a ridge with height $O(x^{-\frac{1}{2}})$. This change in behaviour causes the main problems for the computations based on the earlier mentioned expansions. We give an asymptotic expansion in terms of the error function (or normal distribution function) and related functions. This expansion is valid for x,y large and it is uniformly valid with respect to $|x-y|$, which may range in the interval $[0,\infty)$. The asymptotic problem resembles that for cumulative distribution functions for which the central limit theorem describes the role of the normal distribution function as well. From the cited literature it follows that (1.1) in fact can be viewed as a distribution function.

In LASSEY (1982) a more general function is considered. That is, there the Bessel function of (1.1) shows an argument of the form $2\sqrt{p\xi\eta}$, $p \geqslant 0$. It will be shown in section 6 that our results for (1.1) can easily be generalized for this case, although the limiting form $p \to 1$ may cause some

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computational problems.

In the next section we give a new integral representation for $I(x,y)$ from which in subsequent sections an asymptotic expansion and numerical methods are derived. The estimates and error bounds for the remainders in the expansion show the asymptotic nature of the expansion and they give a sound basis for a numerical algorithm.

2. A NEW INTEGRAL REPRESENTATION FOR (1.1)

The result of this section is the representation

$$I(x,y) = x - \tfrac{1}{2}e^{-x-y}[(x+y)I_0(\omega) + \omega I_1(\omega)] + F(x,y), \tag{2.1}$$

$$F(x,y) = \tfrac{1}{2}\sigma(x-y)\int_\omega^\infty e^{-\sigma t} f(t)dt, \tag{2.2}$$

where I_0, I_1 are modified Bessel functions and

$$f(t) = e^{-t}I_0(t),\ \omega = 2\sqrt{xy}\,,\ \sigma = \frac{(\sqrt{x}-\sqrt{y})^2}{\omega}. \tag{2.3}$$

Before proving this we make some remarks. $I(x,y)$ is symmetric in x and y, so we can (and will) assume that $0 \leqslant x \leqslant y$. In (2.2) we suppose that ω is the large asymptotic parameter and that σ is the uniformity parameter, $\sigma \geqslant 0$. The integral in (2.2) diverges at the diagonal. The factor σ before the integral makes $F(x,y)$ well-defined at $x=y$, the factor $(x-y)$ makes it zero there. By partial integration a convergent integral (at $\sigma=0$) can be obtained, but our asymptotics does not need this. The term with the Bessel functions in (2.1) is exponentially small for large ω, except when $x=y$ where it is $O(x^{-\frac{1}{2}})$. Since also $F(x,y)$ is exponentially small off the diagonal and since $I(x,\infty)=x$ (for both these results see below) it follows that (2.1) is a stable representation for computing $I(x,y)$ when we have a stable algorithm for $F(x,y)$.

2.1. Proof of (2.1), (2.2).

The proof of the above result involves various steps. An essential tool in our approach is the inversion formula for the Laplace integral

$$\int_0^\infty e^{-st}(t/\xi)^{\frac{1}{2}m} I_m(2\sqrt{\xi t}\,)dt = s^{-m-1}e^{\xi/s}, \tag{2.4}$$

which for $m=0$ reads

$$I_0(2\sqrt{\xi\eta}) = \frac{1}{2\pi i}\int_L e^{\xi/s+\eta s}\frac{ds}{s}. \tag{2.5}$$

The contour is a vertical Re $s = const(>0)$ or any contour that can be obtained by deforming it (by using Cauchy's theorem). Observe that (2.4) with $m=0$ gives

$$I(x,\infty) = \int_0^x d\xi = x,\quad I(\infty,y) = y,$$

of which the first one is mentioned above.

By taking for L in (2.5) a small circle around $s=0$ and by substituting (2.5) into (1.1), we obtain the integral

$$I(x,y) = \frac{-1}{2\pi i}\int_L \frac{[e^{-x/(1-1/s)}-1][e^{y(s-1)}-1]}{(s-1)^2}ds.$$

By writing out the product of the nominator, four integrals appear of which three are integrated immediately. Two of them are vanishing:

$$\int_L \frac{e^{y(s-1)}}{(s-1)^2} ds = 0, \quad \int_L \frac{ds}{(s-1)^2} = 0$$

and the third one is

$$\frac{1}{2\pi i} \int_L \frac{e^{-x(1-1/s)}}{(s-1)^2} ds = x.$$

This follows, for instance, from a transformation $s \to 1/s$ and by calculating the residue at $s=1$. So we are left with

$$I(x,y) = x - \frac{e^{-x-y}}{2\pi i} \int_L \frac{e^{x/s+ys}}{(s-1)^2} ds, \tag{2.6}$$

where L is a circle around $s=0$ with radius less than unity. A series expansion follows by writing

$$(1-s)^{-2} = \sum_{m=1}^{\infty} m s^{m-1}, \quad |s| < 1$$

and by using the inversion formula for (2.4). The result is

$$I(x,y) = x - e^{-x-y} \sum_{m=1}^{\infty} m (x/y)^{m/2} I_m(2\sqrt{xy}); \tag{2.7}$$

such expansions appear in LASSEY (1982) for related functions considered there.

By partial integration we have for (2.6)

$$I(x,y) = x + \frac{e^{-x-y}}{2\pi i} \int_L e^{x/s+ys} d \frac{1}{s-1}$$

$$= x - \frac{e^{-x-y}}{2\pi i} \int_L e^{x/s+ys} (y - x/s^2) \frac{ds}{s-1}.$$

By writing $y - x/s^2 = x(s^2-1)/s^2 + (y-x)$ and by using the inversion formula for (2.4) for $m=0,1$ we arrive at

$$I(x,y) = x - xe^{-x-y}[I_0(\omega) + \sqrt{y/x}\, I_1(\omega)] + G(x,y), \tag{2.8}$$

where

$$G(x,y) = \frac{x-y}{2\pi i} e^{-x-y} \int_L \frac{e^{x/s+ys}}{s-1} ds. \tag{2.9}$$

We proceed with $G(x,y)$ and we look for an optimal choice for L. Guided by the saddle point method we take the circle

$$s = \rho e^{i\theta}, \quad \rho = \sqrt{x/y}. \tag{2.10}$$

There is a dominant saddle point at $s=\rho$ and $\mathrm{Im}(x/s+ys) = 0$ along this contour. Observe that saddle point $s = \rho$ and pole $s=1$ coincide when $x=y$. This predicts for the uniform asymptotic expansion an error function as approximant. The theory for this type of phenomena is well developed and we can obtain a uniform expansion directly from (2.9). However we proceed differently since a good error analysis for the remainders in the expansion is more difficult to obtain than for the method that follows.

Integrating (2.9) along the circle $|s| = \rho$ (we suppose temporarily $\rho < 1$) we obtain

$$G(x,y) = \frac{(x-y)e^{-x-y}}{2\pi} \int_0^{2\pi} e^{\omega\cos\theta} \frac{d\theta}{1-\rho^{-1}e^{-i\theta}}.$$

Taking $u = 2\sin\frac{1}{2}\theta$ and separating real and imaginary parts we obtain

$$G(x,y) = \frac{(x-y)e^{-(\sqrt{x}-\sqrt{y})^2}}{2\pi} \int_0^2 e^{-\frac{1}{2}\omega u^2} \frac{2\rho^2-2\rho+u^2}{\rho^2-2\rho+1+\rho u^2} \frac{du}{\sqrt{1-\frac{1}{4}u^2}} \tag{2.11}$$

$$= \tfrac{1}{2}(x-y)e^{-x-y}I_0(\omega) + F(x,y),$$

where ω, ρ are given in (2.3), (2.10) and where

$$F(x,y) = \frac{(x-y)(\rho^2-1)}{2\pi} e^{-(\sqrt{x}-\sqrt{y})^2} \int_0^2 \frac{e^{-\frac{1}{2}\omega u^2}}{(\rho-1)^2+\rho u^2} \frac{du}{\sqrt{1-\frac{1}{4}u^2}}. \tag{2.12}$$

Combining (2.8) and the second line of (2.11) we obtain (2.1). Hence we are finished when we have shown that (2.2) and (2.12) are the same.

Writing $F(x,y)$ in the form (for σ see (2.3))

$$F(x,y)e^{-\omega(\sigma+1)} = \frac{\sigma(x-y)e^{-x-y}}{2\pi} \int_0^2 \frac{e^{-\omega(\sigma+\frac{1}{2}u^2)}}{\sigma+\frac{1}{2}u^2} \frac{du}{\sqrt{1-\frac{1}{4}u^2}},$$

we obtain after differentiation with respect to ω and after integration the final result (2.2). Here we used

$$\lim_{\omega\to\infty} F(x,y) = 0,$$

which easily follows from (2.12), by assuming temporarily that ω is not related to x,y,σ,ρ.

We derived (2.2) under the assumption $x < y$. As remarked earlier we can interprete (2.2) also in the limit $x=y$; it easily follows that $F(x,y)$ is continuous (and analytic) at $x=y$.

2.2. A more general function

LASSEY (1982) considered, among others, the function

$$L(x,y,p) = (1-p)\int_0^x\int_0^y e^{-\xi-\eta}I_0(2\sqrt{p\xi\eta})d\xi d\eta,\ p \geqslant 0, \tag{2.13}$$

which is not a true generalization of (1.1) due to the factor $(1-p)$. At first sight it is not clear why this factor is incorporated (see below, however).

Again, $L(x,y,p)$ is symmetric in x and y. By replacing in (2.5) ξ by ξp we obtain as the analogue of (2.6)

$$L(x,y,p) = 1-e^{xp-1} + \frac{(1-p)e^{-x-y}}{2\pi i}\int_L \frac{e^{xp/s+ys}}{(s-1)(p-s)}\,ds, \tag{2.14}$$

where L is a circle around $s=0$ with radius less than $\min(1,p)$. By writing

$$\frac{p-1}{(s-1)(p-s)} = \frac{1}{s-1} - \frac{1}{s-p}$$

it follows that (2.14) can be written in terms of the function $G(x,y)$ introduced in (2.9). In fact, $L(x,y,p)$ can be written in terms of a few modified Bessel functions and of $I(x,y)$. The limit $p=1$ requires some care, especially when we ask for the computation of $L(x,y,p)/(1-p)$ when $|p-1|$ is small.

3. Uniform asymptotic expansion

We substitute in (2.2) the well-known expansion

$$f(t) \sim \frac{1}{\sqrt{2\pi t}} \sum_{s=0}^{\infty} (-1)^s \frac{A_s}{t^s}, \quad as \quad t \to \infty, \tag{3.1}$$

with

$$A_s = \frac{2^{-s}\Gamma(\frac{1}{2}+s)}{s!\Gamma(\frac{1}{2}-s)}, \quad s = 0,1,2,..., \tag{3.2}$$

and we obtain the formal expansion

$$F(x,y) \sim \frac{\sqrt{\sigma}(x-y)}{2\sqrt{2\pi}} \sum_{s=0}^{\infty} (-1)^s A_s \phi_s \tag{3.3}$$

where

$$\phi_s = \sqrt{\sigma} \int_{\omega}^{\infty} e^{-\sigma t} t^{-s-\frac{1}{2}} dt = \sigma^s \Gamma(\tfrac{1}{2}-s,\sigma\omega). \tag{3.4}$$

Here $\Gamma(a,z)$ is the incomplete gamma function usually defined as

$$\Gamma(a,z) = \int_z^{\infty} e^{-t} t^{a-1} dt \tag{3.5}$$

which reduces to the error function for $a = \frac{1}{2}$. We have

$$\Gamma(\tfrac{1}{2},x^2) = \sqrt{\pi}\,\mathrm{erfc}(x), \quad x \geqslant 0,$$

where

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt. \tag{3.6}$$

So, for a first approximation we have

$$F(x,y) \sim \frac{\sqrt{\sigma}(x-y)}{2\sqrt{2\pi}} \phi_0 = \frac{\sqrt{\sigma}(x-y)}{2\sqrt{2}} \mathrm{erfc}(\sqrt{y} - \sqrt{x}). \tag{3.7}$$

Further terms are obtained from the recursion

$$\Gamma(a+1,z) = a\Gamma(a,z) + z^a e^{-z}. \tag{3.8}$$

So we have for the first few terms in (3.3)

$$\begin{cases} A_0 = 1, & \phi_0 = \sqrt{\pi}\,\mathrm{erfc}(\zeta) \\ A_1 = -\frac{1}{8}, & \phi_1 = 2\sigma[\frac{e^{-\zeta}}{\sqrt{\zeta}} - \phi_0], \\ A_2 = \frac{1}{128}, & \phi_2 = \frac{2\sigma^2}{3}[2\phi_0 + \frac{e^{-\zeta}}{\zeta\sqrt{\zeta}}(1-2\zeta)], \end{cases} \tag{3.9}$$

with $\zeta^2 = \sigma\omega = (\sqrt{y} - \sqrt{x})^2$. Observe that a uniform bound for ϕ_s follows from (3.4) by replacing $e^{-\sigma t}$ by $e^{-\sigma\omega}$:

$$\phi_s \leqslant \frac{e^{-\sigma\omega}}{(s-\frac{1}{2})\omega^{s-\frac{1}{2}}}, \quad s = 1,2,..., \tag{3.11}$$

which shows the asymptotic nature of (3.3). More about this is considered in the next section. Representations for ϕ_1 and ϕ_2 in (3.9) are not stable for large ζ. In fact, early terms in the well-known asymptotic expansion

$$\phi_0 = \sqrt{\pi}\mathrm{erfc}(\sqrt{\zeta}) \sim \frac{e^{-\zeta}}{\sqrt{\zeta}}(1 - \frac{1}{2\zeta} + \frac{3}{4\zeta^2} + ...)$$

will cancell other contributions in, say, ϕ_2. More about this numerical instability in section 5.

4. Error bounds for Remainders

From Olver (1974, p.269) it follows that (3.1) can be replaced by the exact representation

$$f(t) = \frac{1}{\sqrt{2\pi t}}\left\{\sum_{s=0}^{n-1}(-1)^s\frac{A_s}{t^s} + \delta_n\frac{A_n}{t^n}\right\} - \frac{ie^{-2t}}{\sqrt{2\pi t}}\left\{\sum_{s=0}^{m-1}\frac{A_s}{t^s} + \gamma_m\frac{A_m}{t^m}\right\}, \tag{4.1}$$

where, for any $t > 0$, δ_n and γ_m are bounded as follows:

$$|\delta_n| \leqslant 2\chi(n)e^{\pi/(8t)}, \quad |\gamma_m| \leqslant 2e^{1/(4t)}, \tag{4.2}$$

with

$$\chi(n) = \frac{\sqrt{\pi}\Gamma(1+\frac{1}{2}n)}{\Gamma(\frac{1}{2}+\frac{1}{2}n)}. \tag{4.3}$$

Substitution of (4.1) in (2.2) gives an exact version of (3.3) complete with remainders. The second series in (4.1) yields for $m=0$ the contribution

$$\epsilon_0^{(2)} = -\frac{i\sigma(x-y)}{2\sqrt{2\pi}}\int_{\omega}^{\infty} e^{-(\sigma+2)t}\gamma_0 t^{-\frac{1}{2}}dt \tag{4.4}$$

which is estimated by

$$|\epsilon_0^{(2)}| \leqslant \frac{\sigma(y-x)}{\sqrt{2(\sigma+2)}}e^{1/(4\omega)}\mathrm{erfc}(\sqrt{\omega(\sigma+2)}). \tag{4.5}$$

Since now the argument of the error function is bounded away from zero (it equals $\sqrt{x}+\sqrt{y}$) when y and/or x are large, we can use the bound

$$\mathrm{erfc}(z) < e^{-z^2}/z \quad (z>0).$$

We suppose that $(\sqrt{x}+\sqrt{y})^2$ is large enough to make $|\epsilon_0^{(2)}|$ negligible.

The bound for δ_n contains the quantity $\chi(n)$. By using Stirling's formula it follows that

$$\chi(n) = O[(\pi n/2)^{\frac{1}{2}}], \ as\ n \to \infty.$$

A simple upper bound follows from the beta integral for $\chi(n)$ written in the form

$$\chi(n) = \frac{n+1}{2}\int_0^{\infty} e^{-\frac{1}{2}(n+1)t}t^{-\frac{1}{2}}(\frac{e^t-1}{t})^{-\frac{1}{2}}dt.$$

Using $e^t - 1 \geqslant t$ $(t \geqslant 0)$, we obtain

$$\chi(n) \leqslant \sqrt{\pi(n+1)/2}, \quad n > -1.$$

We infer that $F(x,y)$ of (2.20) can be written as (cf.(3.3))

$$F(x,y) = \frac{\sqrt{\sigma}(x-y)}{2\sqrt{2\pi}}\sum_{s=0}^{n-1}(-1)^s A_s\phi_s + \epsilon_n^{(1)} + \epsilon_0^{(2)},$$

where $\epsilon_0^{(2)}$ is considered in (4.4), (4.5) and where $\epsilon_n^{(1)}$ is bounded as follows:

$$|\epsilon_n^{(1)}| \leq \tfrac{1}{2}\sqrt{\sigma(n+1)}\,(y-x)|A_n|\,e^{\pi/(8\omega)}\phi_n.$$

In other words: the remainder $\epsilon_n^{(1)}$ is bounded by the absolute value of the term with $s=n$ in (3.3) apart from the factor

$$\sqrt{2\pi(n+1)}\;e^{\pi/(8\omega)}.$$

This gives a very simple criterion for terminating the asymptotic expansion (3.3).

The above analysis shows that (3.3) is a uniform asymptotic expansion of $F(x,y)$ with ω as a large parameter and $\sigma \in [0,,\infty)$ as a uniformity parameter.

5. On the recursion of the incomplete gamma function

In (3.3) the incomplete gamma functions are needed which can be obtained by the recursion (3.8). As remarked earlier the terms ϕ_s shown in (3.9) exhibit some kind of instability property. For higher terms this instability becomes more important. Although higher terms are required in less numerical precision than the earlier ones, it is appropriate to pay attention to this aspect.

The origin of the instability is (3.8). Observe that we use it in backward direction, with negative a-values. Gautschi (1961) considered the computation of exponential integrals, which are special cases of $\Gamma(a,x)$ with $a=-n$; in the present case we have $a = -n+\frac{1}{2}$, $n = 0,1,\ldots.$ From Gautschi's paper we obtain the following device: To compute

$$\{\phi_s\}_{s=0}^{n},\quad \phi_s \text{ defined in (3.4)} \tag{5.1}$$

where n is appreciably larger than $\zeta = \sigma\omega$ and ζ is larger than five, the subsets

$$\{\phi_s\}_{s=0}^{s_0},\ \{\phi_s\}_{s=s_0}^{n},\quad s_0 = [\zeta].$$

can be computed by recursion with ϕ_{s_0} as starting value in respectively backward and forward direction.

We have not investigated the need of such a device to compute (5.1). We only want to point out that straightforward computation of ϕ_s by using recursion may be an unstable process. Gautschi (1979) gives algorithms for the computation of $\Gamma(a,x)$, also for negative a-values. Amos (1980) gives an algorithm for the computation of exponential integrals. Gautschi's approach of his 1961-paper is also considered in Van der Laan & Temme (1984), with modifications of the error analysis.

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