ELSEVIER

Available at WWW.MATHEMATICSWEB.ORG POWERED BY SCIENCE @ DIRECT®

Journal of Computational and Applied Mathematics 153 (2003) 225–234

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

www.elsevier.com/locate/cam

Computation of the modified Bessel function of the third kind of imaginary orders: uniform Airy-type asymptotic expansion

Amparo Gil[a,*], Javier Segura[b], Nico M. Temme[c]

[a] *Depto. de Matemáticas, Fac. Ciencias, Universidad Autónoma de Madrid, 28049-Madrid, Spain*
[b] *Depto. de Matemáticas, Universidad Carlos III de Madrid, 28911-Leganés, Madrid, Spain*
[c] *CWI, Postbus 94079, 1090 GB Amsterdam, The Netherlands*

Received 7 December 2001

Abstract

The use of a uniform Airy-type asymptotic expansion for the computation of the modified Bessel functions of the third kind of imaginary orders ($K_{ia}(x)$) near the transition point $x = a$, is discussed. In A. Gil et al., Evaluation of the modified Bessel functions of the third kind of imaginary orders, J. Comput. Phys. 17 (2002) 398–411, an algorithm for the evaluation of $K_{ia}(x)$ was presented, which made use of series, a continued fraction method and nonoscillating integral representations. The range of validity of the algorithm was limited by the singularity of the steepest descent paths near the transition point. We show how uniform Airy-type asymptotic expansions fill the gap left by the steepest descent method.

MSC: 33C10; 33F05; 65D20

Keywords: Bessel functions; Nonoscillatory integral representations; Uniform Airy-type asymptotic expansions

0. Introduction

If we can qualify a special function as being important when it appears in mathematical and physical applications, then the modified Bessel function of the third kind of imaginary orders is a quite important one. For instance, this function appears in physical problems such as the solution of the radial Schrödinger equation for exponential potentials, and it also plays an important role in diffraction and hydrodynamics. Besides, $K_{ia}(x)$ solves the Dirichlet problem with boundary conditions

* Corresponding author.
E-mail address: amparo.gil@uam.es (A. Gil).

0377-0427/03/$ - see front matter
PII: S0377-0427(02)00608-8

on a wedge and appears as approximant in certain uniform asymptotic expansion; additionally, $K_{ia}(x)$ is the kernel of the Kantorovich–Lebedev transform.

In spite of its importance, there exists a considerable gap in the numerical libraries regarding its computation. Previous published methods were primarily based on specific quadrature methods relying on oscillatory integral representations. A major concern is the control of relative accuracy when using these integrals, given that the integrals tend to oscillate strongly as the parameters become large.

In [2], we described a strategy for the computation of the K_{ia} function based on series expansions for moderate x, an algorithm based on a continued fraction for hypergeometric functions for moderate a and nonoscillating integral representations when the other two methods failed.

The nonoscillating integral representations result from the application of steepest descent methods, as described in [7]. Given that the differential equation satisfied by the function $K_{ia}(x)$ shows a turning point at $x = a$, where the functions changes from an oscillatory ($x < a$) to a monotonic ($x > a$) behaviour, two different steepest descent integrals arise for these two cases. Unfortunately, it is difficult to match the result from both integrals as x approaches a; in particular, the integral for the oscillating case has a nonsmooth behaviour in this limit caused in part by the peculiar limiting form of the corresponding steepest descent path as $x \to a^+$. As we will show next, this fact sets bounds on the application of the method for large $a \sim x$.

A way of dealing with this problem is by considering approximations which incorporate the behaviour around a simple turning point; that is, considering uniform Airy-type asymptotic expansions.

In this paper we give a brief review of the computational methods described in [2] and we analyse the performance of uniform asymptotic expansions. These combined strategies will be enough to build reliable software for the computation of $K_{ia}(x)$ for a wide range of the parameters. We concentrate on the function $K_{ia}(x)$ though similar methods can be applied for the computation of $K'_{ia}(x)$.

1. Series expansion

Series expansions for $K_{ia}(z)$ and $K'_{ia}(x)$ can be built which properly handle the singularity at $x=0$. The idea, as in [7], is to relate $K_\nu(x)$ with $I_\nu(x)$ to obtain the following expansion:

$$K_\nu(x) = \sum_{k=0}^{\infty} c_k f_k, \tag{1}$$

where

$$f_k = \frac{\pi}{2\sin \nu\pi}\left[\frac{(x/2)^{-\nu}}{\Gamma(k+1-\nu)} - \frac{(x/2)^{\nu}}{\Gamma(k+1+\nu)}\right] \tag{2}$$

and

$$c_k = \left(\frac{x^2}{4}\right)^k \frac{1}{k!} = \frac{x^2}{4}\frac{c_{k-1}}{k}. \tag{3}$$

The coefficients f_k can be computed by forward recursion with starting values f_0 and f_1 which can be evaluated in terms of the Coulomb phase shift [1].

2. Continued fraction method

The Bessel function $K_\nu(x)$ can be expressed in terms of the functions $z_n(x)=U(\nu+\frac{1}{2}+n,2\nu+1,2x)$:

$$K_\nu(x)=\pi^{1/2}(2x)^\nu e^{-x}z_0(x). \tag{4}$$

For the calculation of z_0, a continued fraction representation for the ratio z_1/z_0 is considered:

$$\frac{z_1}{z_0}=\frac{1}{b_1+}\,\frac{a_2}{b_2+}\cdots, \tag{5}$$

where

$$a_{n+1}=-[(n+1/2)^2-\nu^2], \quad b_n=2(n+x) \tag{6}$$

together with a normalization condition [6]:

$$\sum_{n=0}^{\infty}C_n z_n=\left(\frac{1}{2x}\right)^{\nu+1/2}. \tag{7}$$

The computation of the normalization condition can be made in parallel to the evaluation of the continued fraction.

3. Nonoscillating integral representations

In [2], nonoscillating integral representations suitable for computation were built starting from the results in [6].

For the monotonic case ($x>a$) the following representation applies:

$$K_{ia}(x)=\int_0^\infty e^{-x\cosh\tau\cos\sigma-a\sigma}\,d\tau, \tag{8}$$

where $a=x\sin\theta$ and $\sin\sigma=(\sin\theta\,\frac{\tau}{\sinh\tau})$.

This integral representation can be easily computed by using standard quadrature methods [5].

For the oscillatory case ($x<a$), the corresponding integral representation is as follows:

$$\begin{aligned}K_{ia}(x)=e^{-\pi a/2}\Bigg[&\frac{1}{\sinh\pi a}\int_{\mu-\tanh\mu}^{\mu}\left(\cos\chi\sinh\rho+\sin\chi\cosh\rho\,\frac{d\sigma}{d\tau}\right)d\tau\\&-\frac{1}{\sinh\pi a}\int_{\pi}^{3\pi/2}\left(\cos\chi\sinh\rho\,\frac{d\tau}{d\sigma}+\sin\chi\cosh\rho\right)d\sigma\\&+\int_{\mu}^{\infty}e^{-\Psi(\tau)}\left(\cos\chi+\sin\chi\,\frac{d\sigma}{d\tau}\right)d\tau\Bigg],\end{aligned} \tag{9}$$

where $\chi=x\sinh\mu-a\mu$, $\cosh\mu=a/x$, $\mu>0$,

$$\Psi(\tau)=x\cosh\tau\cos\sigma+a(\sigma-\tfrac{1}{2}\pi) \tag{10}$$

and

$$\sin\sigma = \frac{(\tau-\mu)\cosh\mu + \sinh\mu}{\sinh\tau}. \tag{11}$$

The improper integral, as in the monotonic case, can be computed using standard quadrature methods. Regarding the integrals over finite intervals, the second integral in (9) requires the numerical computation of $\tau(\sigma)$ from (11). This inversion can be performed in parallel to the integration.

4. Uniform Airy-type asymptotic expansion

The expansion in terms of Airy functions ($\mathrm{Ai}(z)$ and its derivative $\mathrm{Ai}'(z)$) for $K_{ia}(x)$ is given by (see [4, p. 425])

$$K_{ia}(az) = \frac{\pi e^{-a\pi/2}\phi(\zeta)}{a^{1/3}}\left[\mathrm{Ai}(-a^{2/3}\zeta)\sum_{s=0}^{n}(-)^s\frac{a_s(\zeta)}{a^{2s}} + \frac{\mathrm{Ai}'(-a^{2/3}\zeta)}{a^{4/3}}\sum_{s=0}^{n-1}(-)^s\frac{b_s(\zeta)}{a^{2s}} + \varepsilon_{2n+1}(a,\zeta)\right], \tag{12}$$

where ζ is given by

$$\frac{2}{3}\zeta^{3/2} = \log\frac{1+\sqrt{1-z^2}}{z} - \sqrt{1-z^2}, \quad 0 \leqslant z \leqslant 1,$$

$$\frac{2}{3}(-\zeta)^{3/2} = \sqrt{z^2-1} - \arccos\frac{1}{z}, \quad z \geqslant 1 \tag{13}$$

and

$$\phi(\zeta) = \left(\frac{4\zeta}{1-z^2}\right)^{1/4}, \quad \phi(0) = 2^{1/3}. \tag{14}$$

A bound for the remainder $\varepsilon_{2n+1}(a,\zeta)$ is given in [4, p. 425].

The evaluation of the coefficients near the turning point $z=1$ (which is our region of interest) is performed via Maclaurin series expansions of the quantities ϕ, a_s and b_s [8] in terms of the variable $\eta = 2^{-1/3}\zeta$:

$$\phi(\zeta) = \sum_{t=0}^{\infty}\phi^t\eta^t, \quad a_s(\zeta) = \sum_{t=0}^{\infty}a_s^t\eta^t, \quad b_s(\zeta) = 2^{1/3}\sum_{t=0}^{\infty}b_s^t\eta^t.$$

The coefficients a_s^t, b_s^t can be evaluated through a recurrence relation over t and s:

$$2(2t+1)b_s^t = 2\sum_{r=0}^{t}\psi_r a_s^{t-r} - (t+1)(t+2)a_s^{t+2},$$

$$2(2t+1)a_{s+1}^{t+1} = 2\sum_{r=0}^{t}\psi_r b_s^{t-r} - (t+1)(t+2)b_s^{t+2}, \tag{15}$$

where the quantities ψ_r are the coefficients of the Maclaurin expansion in terms of the variable η of the function

$$\psi(\zeta) = \frac{5}{16\zeta^2} + \frac{\zeta z^2(z^2+4)}{4(z^2-1)^3}:$$

$$\psi(\zeta) = 2^{1/3}\sum_{r=0}^{\infty}\psi_r\eta^r. \tag{16}$$

To obtain a_s^0, $s \geqslant 1$ (it is known that $a_0(\zeta) = 1$) one can use the following relation:

$$2a_{s+1}^0 = -\sum_{r=1}^{s} a_r^0 a_{s+1-r}^0 - \sum_{r=0}^{s}[a_r^0 b_{s-r}^1 - a_r^1 b_{s-r}^0], \quad s = 0,1,2,\ldots . \tag{17}$$

From the first relation of (15) it is clear than $b_0^t = \psi_t/(2t+1)$, $t = 0,1,2,\ldots$.

In the appendix we provide a Maple code for the computation of the coefficients of the Maclaurin expansions of the functions $z(\zeta)$, $\phi(\zeta)$, $\psi(\zeta)$ as well as $a_s(\zeta)$, $b_s(\zeta)$ for $s = 0,\ldots,3$.

5. Numerical aspects

Fig. 1 shows the regions where series, the continued fraction method and nonoscillating integral representations can be applied. The shaded regions represent the values of the parameters for which series and the CF method agree with steepest descent integrals for an accuracy of 10^{-9}. In the unshaded regions neither series nor CF can be applied and we are left with the nonoscillating integrals.

The integrals considered, and in particular, the integral for the oscillatory case ($x < a$) become difficult to compute as x approaches a. This is related to the peculiar limiting form of the steepest descent path and the rapid variation of the first two integrands in (9) at the extremes of integration [2].

In order to illustrate more clearly the loss of precision as $a \to x^+$ it is convenient to look closer to the comparison of the CF versus integrals close to $x = a$. Fig. 2 shows such analysis. A sweep

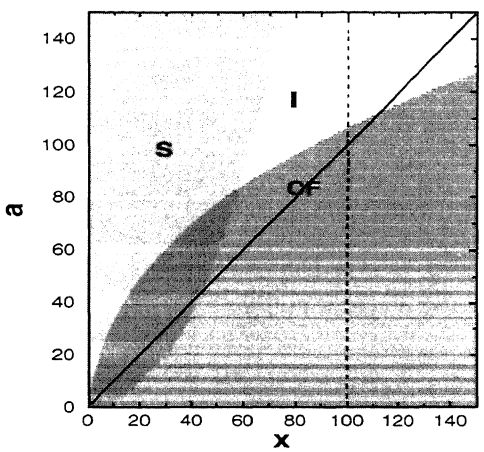

Fig. 1. Regions where series and the continued fraction method coincide with nonoscillating integrals for a precision better than 10^{-9}. For $x < 100$, the regions where each of these approaches can be safely applied is labeled with different letters.

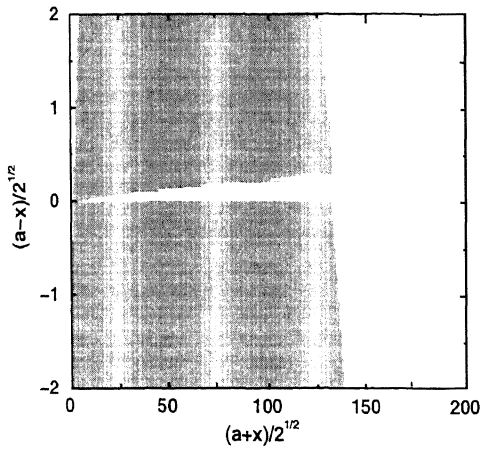

Fig. 2. Comparison of the continued fraction method and integrals for a precision of 10^{-9}.

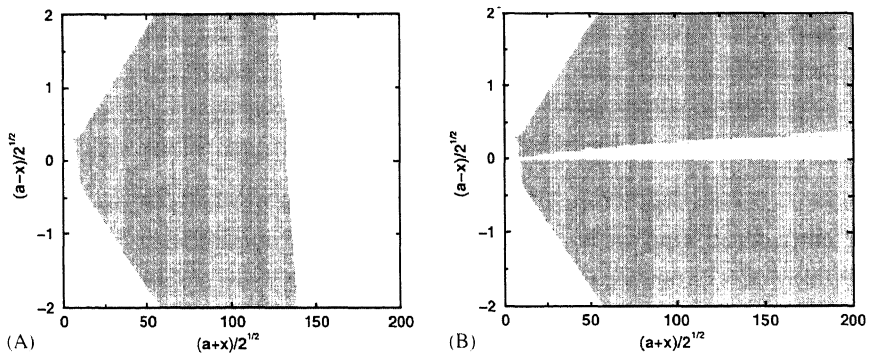

Fig. 3. (A) Comparison of the continued fraction method and the uniform asymptotic expansion for a precision of 10^{-9}. (B) Comparison of the integrals and the uniform asymptotic expansion for a precision of 10^{-9}.

of parameter values is performed around $x = a$ using as axis $(x + a)/\sqrt{2}$ and $(a - x)/\sqrt{2}$. Indeed, we observe some discrepancies for small $a - x > 0$.

For this reason, the algorithm based on series, CF and integrals had to be limited to $x < 100$ in order to avoid the consideration of the integral for the oscillatory case for x too close to a. This is, however, a broad range if one considers that for such high values the function drops to values of the order of 10^{-45} at most.

In any case, the performance and range of application can be improved by using Airy-type uniform asymptotic expansions [4,8], as we have discussed before. Fig. 3A shows the comparison between the asymptotic expansion and the CF while Fig. 3B shows the comparison between the asymptotic expansion and the integral representations; the same rotation of axes as in Fig. 2 is considered. Four a_s and b_s coefficients are considered, expanded up to power 4 (at most) in ζ. For the computation of the Airy function we use an algorithm based on series, Gaussian quadrature and asymptotic expansions [3].

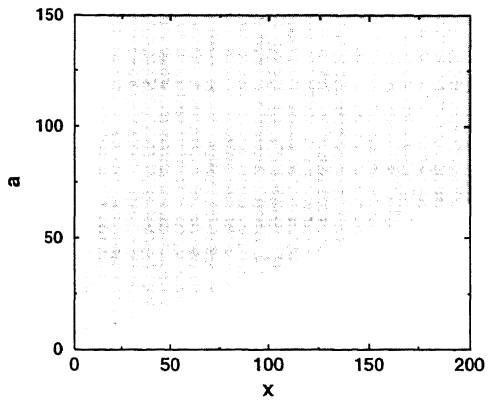

Fig. 4. Comparison of the integrals and the uniform asymptotic expansion for a precision of 10^{-9} and for 20 coefficients in the series expansion of a_s, b_s, $s = 0, 1, 2, 3$. The accuracy problem of the integral as $x \to a^+$ is not observed (but it is present) due to the large range displayed in both axis.

We observe that this is enough to safely avoid the computation of the integral in the compromised region and that, therefore, the use of asymptotics helps in increasing the range of computation. In this way, one can safely and accurately compute the function $K_{ia}(x)$ with the only practical limitation of the underflow capabilities of the computer in use.

The range of application of the uniform asymptotic expansion can be extended both by considering further a_s and b_s coefficients and further terms in the expansions of these coefficients. For moderate a the CF method is an accurate and efficient method; therefore, adding more a_s and b_s coefficients would not improve the performance of the algorithm. However, it could be interesting to consider more terms in the expansion of the coefficients in order to enlarge the region around $x = a$ where asymptotics can be applied.

Fig. 4 shows the region of coincidence of the asymptotic expansion and the integrals when up to 20 coefficients in the Taylor series for the a_s and b_s coefficients are considered (we again take $s=0, 1, 2, 3$). In this case, power series, asymptotic expansions and the CF method suffice to compute $K_{ia}(x)$ in the a–x plane.

The four methods of computation described are therefore such that for any point in the $a-x$, there are at least two methods that can be applied, except for a tiny region above the line $x = a$ (where we can rely on asymptotics). Integrals have the largest range of applicability, followed by uniform asymptotics, the CF method and power series. This overlapping will be important in order to build reliable codes with accuracy well under control; the selection of methods in the different regions of parameter space will be determined by the reachable accuracy and the speed of computation.

Acknowledgements

A. Gil acknowledges financial support for Alexander von Humboldt Foundation. J. Segura acknowledges financial support from DAAD.

Appendix

```
#  Maple code for the computation of the coefficients used in
#  the Airy-type asymptotic expansions
#  Ref.: N.M. Temme, ''Numerical Algorithms for uniform Airy-type
#                    asymptotic expansions''
#                    Numer. Algorithms 15, No.2 (1997) 207-225.
   restart;
   readlib(coeftayl);
#  up: number of terms in the expansion of z(zeta). The number of coefficients
#      in the rest of expansions is smaller than up.
   up:=30;
   psi:=5/32/eta^2+eta*z2*(z2+4)/4/(z2-1)^3;
   phi:=(2*eta/(1-z2))^(1/4);
   v:=2*eta*z2-(1-z2)*zd^2;
#  Maclaurin expansions for the functions z(zeta), psi(zeta), phi(zeta)
   zn[0]:=1; zn[1]:=-1;
   z:=sum(zn[k]*eta^k,k=0..up);
   zd:=diff(z,eta);
   z2:=normal(taylor(z^2,eta=0,up-1));
   vt:=normal(taylor(v,eta=0,up));
   for j from 2 to up-2 do
       p:=normal(coeftayl(vt,eta=0,j));
       zn[j]:=normal(solve(p=0,zn[j]))
   od;
   for j from 0 to up-2 do
       lprint('zn[',j,']:=',zn[j],';')
   od;
   psit:=normal(taylor(psi, eta=0,up-1));
   for j from 0 to up-7 do
       psin[j]:=coeftayl(psit,eta=0,j)
   od;
   for j from 0 to up-7 do
       lprint('psin[',j,']:=',psin[j],';')
   od;
   phit:=normal(taylor(phi,eta=0,up-2));
   for j from 0 to up-3 do
       phin[j]:=coeftayl(phit,eta=0,j)
   od;
   for j from 0 to up-3 do
       lprint('phin[',j,']:=',phin[j],';')
   od;
#  Computation of the coefficients a_s^t, b_s^t for s=0 to s=4.
   s:=0; up:=up-7;
```

```
ast[s,0]:=1;
for t from 1 to up do ast[s,t]:=0 od;
for t from 0 to up do bst[s,t]:=psin[t]/(2*t+1) od;
s:=1;
for t from 0 to up-2 do
    u:=0;
    for k from 0 to t do u:=u+bst[s-1,t-k]*psin[k] od;
    ast[s,t+1]:=(2*u-(t+1)*(t+2)*bst[s-1,t+2])/(2*(t+1))
od;
u:=-(ast[0,0]*bst[s-1,1]-ast[0,1]*bst[s-1,0]);
for j from 1 to s-1 do
    u:=u-ast[j,0]*ast[s-j,0]-(ast[j,0]*bst[s-1-j,1]-ast[j,1]*bst[s-1-j,0]);
od;
ast[s,0]:=u/2;
for t from 0 to up-3 do
    u:=0;
    for k from 0 to t do u:=u+ast[s,t-k]*psin[k] od;
    bst[s,t]:=(2*u-(t+1)*(t+2)*ast[s,t+2])/(2*(2*t+1))
od;
s:=2; up:=up-3;
for t from 0 to up-2 do
    u:=0;
    for k from 0 to t do u:=u+bst[s-1,t-k]*psin[k] od;
    ast[s,t+1]:=(2*u-(t+1)*(t+2)*bst[s-1,t+2])/(2*(t+1))
od;
u:=-(ast[0,0]*bst[s-1,1]-ast[0,1]*bst[s-1,0]);
for j from 1 to s-1 do
    u:=u-ast[j,0]*ast[s-j,0]-(ast[j,0]*bst[s-1-j,1]-ast[j,1]*bst[s-1-j,0]);
od;
ast[s,0]:=u/2;
for t from 0 to up-3 do
    u:=0;
    for k from 0 to t do u:=u+ast[s,t-k]*psin[k] od;
    bst[s,t]:=(2*u-(t+1)*(t+2)*ast[s,t+2])/(2*(2*t+1))
od;
s:=3; up:=up-3;
for t from 0 to up-2 do
    u:=0;
    for k from 0 to t do u:=u+bst[s-1,t-k]*psin[k] od;
    ast[s,t+1]:=(2*u-(t+1)*(t+2)*bst[s-1,t+2])/(2*(t+1))
od;
u:=-(ast[0,0]*bst[s-1,1]-ast[0,1]*bst[s-1,0]);
for j from 1 to s-1 do
    u:=u-ast[j,0]*ast[s-j,0]-(ast[j,0]*bst[s-1-j,1]-ast[j,1]*bst[s-1-j,0);
```

```
od;
ast[s,0]:=u/2;
for t from 0 to up-3 do
    u:=0;
    for k from 0 to t do u:=u+ast[s,t-k]*psin[k] od;
    bst[s,t]:=(2*u-(t+1)*(t+2)*ast[s,t+2])/(2*(2*t+1))
od;
s:=4; up:=up-3;
for t from 0 to up-2 do
    u:=0;
    for k from 0 to t do u:=u+bst[s-1,t-k]*psin[k] od;
    ast[s,t+1]:=(2*u-(t+1)*(t+2)*bst[s-1,t+2])/(2*(t+1))
od;
u:=-(ast[0,0]*bst[s-1,1]-ast[0,1]*bst[s-1,0]);
for j from 1 to s-1 do
    u:=u-ast[j,0]*ast[s-j,0]-(ast[j,0]*bst[s-1-j,1]-ast[j,1]*bst[s-1-j,0]);
od;
ast[s,0]:=u/2;
for t from 0 to up-3 do
    u:=0;
    for k from 0 to t do u:=u+ast[s,t-k]*psin[k] od;
    bst[s,t]:=(2*u-(t+1)*(t+2)*ast[s,t+2])/(2*(2*t+1))
od;
```

References

[1] W.J. Cody, K.E. Hillstrom, Chebyshev approximations for the Coulomb phase shift, Math. Comput. 24 (111) (1970) 671–677.

[2] A. Gil, J. Segura, N.M. Temme, Evaluation of the modified Bessel functions of the third kind of imaginary orders, J. Comput. Phys. 17 (2002) 398–411.

[3] A. Gil, J. Segura, N.M. Temme, Computing complex Airy functions by numerical quadrature, Numer. Algorithms 30 (2002) 11–23.

[4] F.J.W. Olver, Asymptotics and Special Functions, Reprinted in 1997 by AK Peters.

[5] R. Piessens, E. De Doncker, Subroutine DQAGIE, obtained from SLATEC Public Domain Library.

[6] N.M. Temme, On the numerical evaluation of the modified Bessel function of the third kind, J. Comput. Phys. 19 (3) (1975) 324–337.

[7] N.M. Temme, Steepest descent paths for integrals defining the modified Bessel functions of imaginary order, Methods Appl. Anal. 1 (1994) 14–24.

[8] N.M. Temme, Numerical algorithms for uniform Airy-type asymptotic expansions, Numer. Algorithms 15 (2) (1997) 207–225.

For further reading

I.J. Thompson, A.R. Barnett, Modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ of real order and complex argument, to selected accuracy, Comput. Phys. Comm. 47 (2–3) (1987) 245–257.