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Computing special functions by using quadrature rules

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The usual tools for computing special functions are power series, asymptotic expansions, continued fractions, differential equations, recursions, and so on. Rather seldom are methods based on quadrature of integrals. Selecting suitable integral representations of special functions, using principles from asymptotic analysis, we develop reliable algorithms which are valid for large domains of real or complex parameters. Our present investigations include Airy functions, Bessel functions and parabolic cylinder functions. In the case of Airy functions we have improvements in both accuracy and speed for some parts of Amos's code for Bessel functions.

Keywords: numerical computation of special functions, numerical quadrature, steepest descent method, saddle point method, Airy functions, Bessel functions

AMS subject classification: 65D20, 65D32, 33C10, 33F05, 41A60

1. Introduction

We start with a simple example in which an oscillatory integral can be transformed into a stable representation. Consider the integral

$$F(\lambda) = \int_{-\infty}^{\infty} \mathrm{e}^{-t^2+2\mathrm{i}\lambda t}\,\mathrm{d}t = \sqrt{\pi}\mathrm{e}^{-\lambda^2}. \tag{1.1}$$

Taking $\lambda = 10$ we get

$$F(\lambda) \doteq 0.6593662990 \cdot 10^{-43}. \tag{1.2}$$

When we ask a computer algebra system to do a numerical evaluation of the integral, without using the exact answer in (1.1) and with standard 10 digits accuracy, we obtain

$$F(\lambda) \doteq 0.24 \cdot 10^{-12}. \tag{1.3}$$

We see that this simple integral, with strong oscillations, cannot be evaluated correctly. Increasing the accuracy from 10 to 50 digits we obtain the answer

$$F(\lambda) \doteq 0.65936629906 \cdot 10^{-43}, \tag{1.4}$$

the first 8 digits being correct. Observe that we can shift the path of integration upwards until we reach the point $t = i\lambda$, the saddle point, and we write

$$F(\lambda) = \int_{-\infty}^{\infty} \mathrm{e}^{-(t-\mathrm{i}\lambda)^2-\lambda^2}\,\mathrm{d}t = \mathrm{e}^{-\lambda^2} \int_{-\infty}^{\infty} \mathrm{e}^{-s^2}\,\mathrm{d}s. \tag{1.5}$$

Now the saddle point is at $s = 0$, we integrate through this point along a path where no oscillations occur, a *steepest descent path.* Moreover the small factor $\mathrm{e}^{-\lambda^2}$ that causes the main problems in the standard quadrature method, is now in front of the s-integral.

Similar methods can be applied to more complicated functions, in particular to a wide class of special functions from mathematical physics. Much software has been developed for many of these functions, but for large parameters the software is not at all complete and reliable, in particular when the parameters are large and complex.

We have come to the conclusion that methods based on asymptotic analysis are important for evaluating integrals by quadrature. Choosing suitable paths of integration and scaling the functions by separating dominant factors are important steps in these methods.

In this paper we discuss the basic elements of the quadrature method and we indicate which group of special functions presently has our attention.

2. Airy functions

Airy functions are solutions of the differential equation

$$\frac{\mathrm{d}^2 w}{\mathrm{d}w^2} - xw = 0. \tag{2.1}$$

Asymptotic forms for large complex z are

$$\begin{aligned} \mathrm{Ai}(z) &= \frac{1}{2\sqrt{\pi}} z^{-1/4} \mathrm{e}^{-\zeta}\left[1 + \mathrm{O}\left(z^{-3/2}\right)\right], \quad |\mathrm{ph}\, z| < \pi, \\ \mathrm{Bi}(z) &= \frac{1}{\sqrt{\pi}} z^{-1/4} \mathrm{e}^{\zeta}\left[1 + \mathrm{O}\left(z^{-3/2}\right)\right], \quad |\mathrm{ph}\, z| < \frac{1}{3}\pi, \end{aligned} \tag{2.2}$$

where ζ is defined by $\zeta = \frac{2}{3} z^{3/2}$. Also, for $|\mathrm{ph}\, z| < \frac{2}{3}\pi$,

$$\begin{aligned} \mathrm{Ai}(-z) &\sim \frac{1}{\sqrt{\pi}} z^{-1/4} \left[\cos\left(\zeta - \frac{1}{4}\pi\right) + \mathrm{O}\left(\frac{1}{\zeta}\right)\right], \\ \mathrm{Bi}(-z) &\sim -\frac{1}{\sqrt{\pi}} z^{-1/4} \left[\sin\left(\zeta - \frac{1}{4}\pi\right) + \mathrm{O}\left(\frac{1}{\zeta}\right)\right]. \end{aligned} \tag{2.3}$$

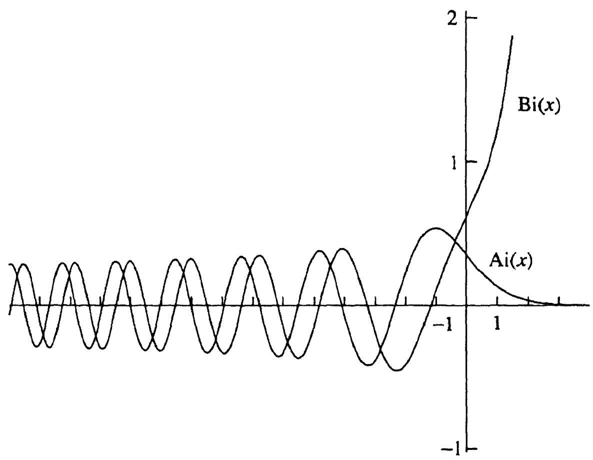

Figure 1. Graphs of Airy functions $\mathrm{Ai}(x)$ and $\mathrm{Bi}(x)$.

One integral representation is (see [1, p. 447])

$$\mathrm{Ai}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\cos\left(\frac{1}{3}t^3 + xt\right)\mathrm{d}t, \quad x \in \mathbb{R}. \tag{2.4}$$

This integral is not a suitable representation for numerical quadrature, in particular when x is positive. In that case $\mathrm{Ai}(x)$ is exponentially small, whereas $\mathrm{Ai}(x)$ is oscillating for $x < 0$. We can explain this different behaviour by pointing out the role of the real stationary points $\pm\sqrt{-x}$, $x < 0$ of $\cos(\frac{1}{3}t^3 + xt)$ in the integral representation of $\mathrm{Ai}(x)$. See figure 2.

A much better representation is used by Gautschi in [4]:

$$\mathrm{Ai}(z) = \frac{z^{-1/4}\mathrm{e}^{-\zeta}}{\sqrt{\pi}\,\Gamma(5/6)}\int_0^{\infty}\left(1 + \frac{t}{2\zeta}\right)^{-1/6} t^{-1/6}\mathrm{e}^{-t}\,\mathrm{d}t, \tag{2.5}$$

where

$$\zeta = \frac{2}{3}z^{3/2}, \quad |\mathrm{ph}\,\zeta| < \pi \quad \Longrightarrow \quad |\mathrm{ph}\,z| < \frac{2}{3}\pi. \tag{2.6}$$

Now the dominant term $\mathrm{e}^{-\zeta}$ is in front of the integral; the integral itself is monotonic, if $z > 0$.

For evaluating the integral in (2.5), Gautschi suggests for $z \geqslant 2$ a generalized Gauss–Laguerre quadrature rule with Laguerre parameter $\alpha = -\frac{1}{6}$, and reports that a 22-point Gauss rule yields double-precision accuracy and a 83-point formula quadruple-precision accuracy.

We have investigated this integral for complex values also. We found that a 40-point Gauss rule yields 13D–14D accuracy in the sector

$$|\theta| \leqslant \frac{1}{2}\pi, \qquad |z| \geqslant 1, \quad \theta = \mathrm{ph}\,z. \tag{2.7}$$

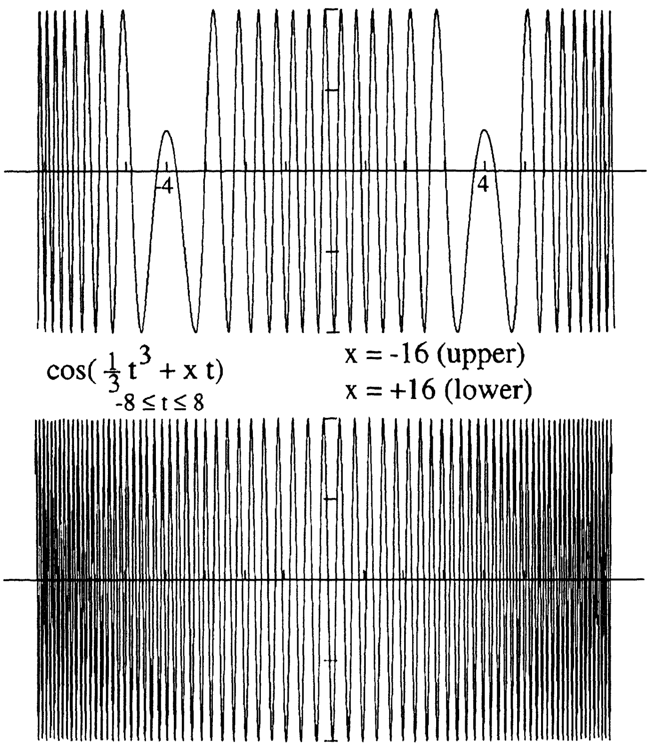

Figure 2. Graphs of $\cos(\frac{1}{3}t^3 + xt)$, $x = -16$, with stationary points at $t = \pm\sqrt{-x}$ (top) and with $x = 16$ (bottom), with no stationary points inside the shown interval.

Outside this sector, in particular, when $\theta \to \pm\frac{2}{3}\pi$, the singularity at $t = -2\zeta$ reaches the positive real axis, and accuracy is therefore lost.

By turning the path of integration we can always avoid this situation. In fact, if $|\theta| \in [\frac{1}{2}\pi, \frac{2}{3}\pi]$ we turn the path, and use the representation

$$\operatorname{Ai}(z) = \left(\frac{e^{i\tau}}{\cos\tau}\right)^{5/6} \frac{z^{-1/4}e^{-\zeta}}{\sqrt{\pi}\,\Gamma(5/6)} \int_0^\infty e^{-it\tan\tau}\left(1 + \frac{t}{2\zeta'}\right)^{-1/6} t^{-1/6}e^{-t}\,dt, \tag{2.8}$$

where

$$\zeta' = \cos\tau e^{-i\tau}\zeta, \qquad \tau = \frac{3}{2}\left(\theta - \frac{1}{2}\pi\right), \tag{2.9}$$

τ being the angle for turning the path of integration.

In this way one Gauss rule can be used for the complete sector $|\theta| \leqslant \frac{2}{3}\pi$. Outside this sector a connection formula for the Airy functions can be used:

$$\operatorname{Ai}(z) = -e^{-2\pi i/3}\operatorname{Ai}\left(e^{-2\pi i/3}z\right) - e^{2\pi i/3}\operatorname{Ai}\left(e^{2\pi i/3}z\right). \tag{2.10}$$

For large values of z we use the asymptotic expansion and for small values Taylor series.

Comparing this algorithm with [2], an important package for complex Bessel functions, we notice several improvements. In some cases Amos's code is less accurate than ours, and in some cases we also have a faster code. More details are given in the papers [8,10].

3. The trapezoidal rule

Gauss quadrature is one example of evaluating integrals. It has a very good performance for various types of integrals over real intervals. One of the drawbacks is that it is not very flexible in algorithms when we want adjustable precision.

We need zeros and weights of a certain class of orthogonal polynomials. For high precision algorithms computing these numbers in advance may be time consuming and/or not reliable.

The n-point extended trapezoidal rule

$$\int_a^b f(t)\,\mathrm{d}t = \frac{1}{2}h\big[f(a)+f(b)\big] + h\sum_{j=1}^{n-1} f(hj) + R_n, \quad h = \frac{b-a}{n}, \tag{3.1}$$

is more flexible, because we do not need precomputed zeros and weights; for this rule these numbers are trivial.

The error term has the form

$$R_n = -\frac{nh^3}{12} f''(\xi), \tag{3.2}$$

for some point $\xi \in (a,b)$, and for functions with continuous second derivative.

Example 1 (The Bessel function $J_0(x)$). We take as an example the Bessel function

$$\pi J_0(x) = \int_0^\pi \cos(x\sin t)\,\mathrm{d}t = h + h\sum_{j=1}^{n-1}\cos\big[x\sin(hj)\big] + R_n, \tag{3.3}$$

where $h = \pi/n$, and use this rule for $x = 5$. We have the following results:

n	R_n
4	$-0.12 \cdot 10^{-0}$
8	$-0.48 \cdot 10^{-6}$
16	$-0.11 \cdot 10^{-21}$
32	$-0.13 \cdot 10^{-62}$
64	$-0.13 \cdot 10^{-163}$
128	$-0.53 \cdot 10^{-404}$

We observe that the error R_n is much smaller than the upper bound that can be obtained from (3.2). The explanation comes from the periodicity in the integral for the Bessel function. In fact we have:

Theorem 1. If $f(t)$ is periodic and has a continuous kth derivative, and if the integral is taken over a period, then

$$|R_n| \leqslant \frac{\text{constant}}{n^k}. \tag{3.4}$$

In the case of the Bessel function, we can take any k in this theorem, and we infer that now the error is exponentially small.

For more details we refer to [3]. In [13, Vol. II, p. 218] this Bessel function integral is considered in detail, and from this reference and [12] we derive an upper bound for R_n:

$$|R_n| \leqslant 2\mathrm{e}^{x/2}\frac{(x/2)^{2n}}{(2n)!}, \tag{3.5}$$

which is quite realistic for the value of x we chose.

Another example is the Bessel function integral for general order

$$J_\nu(x) = \frac{1}{2\pi \mathrm{i}}\int_C \mathrm{e}^{-x\sinh t+\nu t}\,\mathrm{d}t, \tag{3.6}$$

where C starts at $-\infty - \mathrm{i}\pi$ and terminates at $\infty + \mathrm{i}\pi$; see [15, p. 222]. On this contour oscillations will occur, but we will select a special contour that is free of oscillations for the case $x \leqslant \nu$.

We write $\nu = x\cosh\mu$, $\mu \geqslant 0$. The saddle point of $-x\sinh t + \nu t = -x(\sinh t - t\cosh\mu)$ occurs at $t = \mu$, and at this saddle point the imaginary part of $-x\sinh t + \nu t$ equals zero. A path free of oscillations (a steepest descent path through the saddle point) can be described by the equation $\Im(-x\sinh t + \nu t) = 0$. Writing $t = \sigma + \mathrm{i}\tau$ we obtain for the path the equation

$$\cosh\sigma = \cosh\mu\frac{\tau}{\sin\tau}, \qquad -\pi < \tau < \pi, \tag{3.7}$$

and on this path we have

$$\Re(-x\sinh t + \nu t) = -x(\sinh\sigma\cos\tau - \sigma\cosh\mu). \tag{3.8}$$

Integrating with respect to τ, using $\mathrm{d}t/\mathrm{d}\tau = (\mathrm{d}\sigma/\mathrm{d}\tau + \mathrm{i})$ (where $\mathrm{d}\sigma/\mathrm{d}\tau$ is an odd function of τ), we obtain

$$J_\nu(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-x(\sinh\sigma\cos\tau-\sigma\cosh\mu)}\,\mathrm{d}\tau, \qquad 0 < x \leqslant \nu. \tag{3.9}$$

The integrand is analytic and vanishes with all its derivatives at the points $\pm\pi$. We can interpret the integrand as being a periodic C^∞ function with period 2π, and consider theorem 1. Again, the error in the trapezoidal rule is exponentially small.

When $\nu \gg x$ the Bessel function becomes very small and we can take the dominant part $\mathrm{e}^{-x(\sinh\mu-\mu\cosh\mu)}$ in front of the integral. When $x \geqslant \nu$ (the oscillatory case), the Bessel function can be represented in a similar way, now by using two integrals (coming from the Hankel functions).

Our main conclusion of this section is that the trapezoidal rule may be very efficient and accurate when dealing with a certain class of integrals. Smoothness and periodicity of the integrand are the key properties here.

4. The trapezoidal rule on $\mathbb{R}$

In the previous section we considered integrals over finite intervals. For integrals over $\mathbb{R}$ the trapezoidal rule may again be very efficient and accurate.

We consider

$$\int_{-\infty}^{\infty} f(t)\,\mathrm{d}t = h\sum_{j=-\infty}^{\infty} f(hj+d) + R_d(h) \tag{4.1}$$

where $h > 0$ and $0 \leqslant d < h$.

We consider this rule for functions analytic in a strip of width $2a > 0$ around $\mathbb{R}$:

$$G_a = \{z = x + \mathrm{i}y \mid x \in \mathbb{R},\ -a < y < a\}. \tag{4.2}$$

Let H_a denote the linear space of functions $f : G_a \to \mathbb{C}$, which are bounded in G_a and for which

$$\lim_{x\to\pm\infty} f(x+\mathrm{i}y) = 0 \tag{4.3}$$

(uniformly in $|y| \leqslant a$) and

$$M_{\pm a}(f) = \int_{-\infty}^{\infty} \bigl|f(x \pm \mathrm{i}a)\bigr|\,\mathrm{d}x = \lim_{b\uparrow a}\int_{-\infty}^{\infty}\bigl|f(x\pm \mathrm{i}b)\bigr|\,\mathrm{d}x < \infty. \tag{4.4}$$

Theorem 2. Let $f \in H_a$ for some $a > 0$. Then $R_d(h)$ of (4.1) satisfies

$$R_d(h) = \int_{-\infty}^{\infty} \frac{f(x+\mathrm{i}y)\,\mathrm{d}x}{1-\exp[-2\pi\mathrm{i}(x+\mathrm{i}y-d)/h]} + \int_{-\infty}^{\infty} \frac{f(x-\mathrm{i}y)\,\mathrm{d}x}{1-\exp[2\pi\mathrm{i}(x-\mathrm{i}y-d)/h]} \tag{4.5}$$

for any y with $0 < y < a$. Moreover, if f is even, then

$$\bigl|R_d(h)\bigr| \leqslant \frac{\mathrm{e}^{-\pi a/h}}{\sinh(\pi a/h)} M_a(f), \tag{4.6}$$

where $M_a(f)$ is given in (4.4).

Proof. The proof is based on residue calculus; see [13, Vol. II, p. 217]. □

Example 2 (Modified Bessel function $K_0(x)$). Consider the modified Bessel function

$$K_0(x) = \frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh t}\, dt. \tag{4.7}$$

We have, with $d = 0$,

$$e^x K_0(x) = \frac{1}{2}h + h\sum_{j=1}^{\infty} e^{-x(\cosh(hj)-1)} + R_0(h). \tag{4.8}$$

For $x = 5$ and several values of h we obtain (j_0 denotes the number of terms used in the series in (4.1)

h	j_0	$R_0(h)$
1	2	$-0.18 \cdot 10^{-1}$
1/2	5	$-0.24 \cdot 10^{-6}$
1/4	12	$-0.65 \cdot 10^{-15}$
1/8	29	$-0.44 \cdot 10^{-32}$
1/16	67	$-0.19 \cdot 10^{-66}$
1/32	156	$-0.55 \cdot 10^{-136}$
1/64	355	$-0.17 \cdot 10^{-272}$

We see in this example that halving the value of h gives a doubling of the number of correct significant digits (and, roughly speaking, a doubling of the number of terms needed in the series). When programming this method, observe that when halving h, previous function values can be used. Details on error bounds for the remainder in this example follow from [12].

5. Computing special functions

In recent and future publications we consider, in particular, the following functions:

1. Airy functions. The Gauss–Laguerre method mentioned earlier is fine for fixed precision. For adjustable precision it is better to use complex contour integrals. Saddle point methods from asymptotics are used to bring the integral in a standard from suitable for applying the trapezoidal rule.
2. Inhomogeneous Airy functions, that is, solutions of the equation

$$\frac{d^2 w}{dx^2} - xw = \pm\frac{1}{\pi}. \tag{5.1}$$

See [5] for the construction of non-oscillating integral representations for these functions. In [9] numerical algorithms based on these integrals are given.

3. Modified Bessel functions of imaginary order. The prototype is

$$K_{ia}(x) = \int_0^{\infty} e^{-x\cosh t}\cos at\, dt \tag{5.2}$$

for $a \geqslant 0, x > 0$. These integrals are difficult to evaluate for large values of a and x. Uniform asymptotic expansions can be used, in particular when $a \sim x$, but for numerical evaluations it seems better to use integral representations. Again, saddle point methods give a standard form, and we can apply the trapezoidal rule for infinite integrals. See also [6,7,14].

4. Parabolic cylinder functions. One example is

$$U(a,z) = \frac{\mathrm{e}^{(1/4)z^2}}{\mathrm{i}\sqrt{2\pi}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{e}^{-zs+(1/2)s^2} s^{-a-1/2}\,\mathrm{d}s, \quad c > 0. \tag{5.3}$$

These functions are related with confluent hypergeometric functions (Kummer or Whittaker functions). They are difficult to compute when the parameters are large (and certainly when they are complex). No reliable software is available for large values of the parameters. Again, the integral can be transformed into a suitable real integral and the trapezoidal rule can be applied for constructing stable and efficient algorithms; see [11].

6. Complex contours

Although we now have an efficient quadrature method for complex Airy functions based on Gauss–Laguerre quadrature, we explain how a complex contour integral for the Airy function can be transformed into a suitable real integral for applying the trapezoidal rule of section 4. This gives a very flexible and efficient algorithm with adjustable precision.

We consider

$$\mathrm{Ai}(z) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} \mathrm{e}^{(1/3)w^3 - zw}\,\mathrm{d}w, \tag{6.1}$$

where $\mathrm{ph}\, z \in [0, \frac{2}{3}\pi]$ and $\mathcal{C}$ is a contour starting at $\infty\mathrm{e}^{-\mathrm{i}\pi/3}$ and terminating at $\infty\mathrm{e}^{+\mathrm{i}\pi/3}$ (in the valleys of the integrand).

Let

$$\phi(w) = \frac{1}{3}w^3 - zw. \tag{6.2}$$

The saddle points are $w_0 = \sqrt{z}$ and $-w_0$ and follow from solving $\phi'(w) = w^2 - z = 0$.

The saddle point contour (the path of steepest descent) that runs through the saddle point w_0 is defined by

$$\Im[\phi(w)] = \Im[\phi(w_0)]. \tag{6.3}$$

We write

$$z = x + \mathrm{i}y = r\mathrm{e}^{\mathrm{i}\theta}, \qquad w = u + \mathrm{i}v, \qquad w_0 = u_0 + \mathrm{i}v_0. \tag{6.4}$$

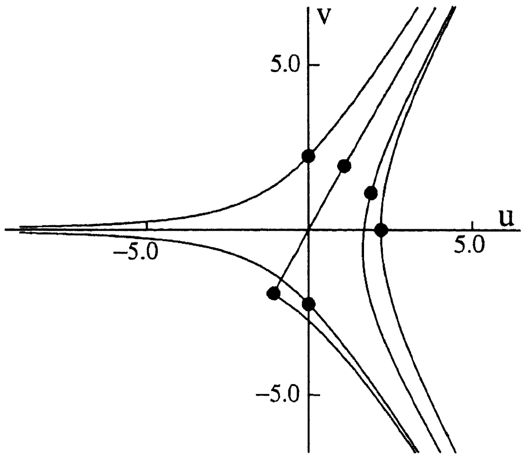

Figure 3. Saddle point contours for $\theta = 0, \frac{1}{3}\pi, \frac{2}{3}\pi, \pi$ and $r = 5$.

Then

$$u_0 = \sqrt{r}\cos\frac{1}{2}\theta, \qquad v_0 = \sqrt{r}\sin\frac{1}{2}\theta, \qquad x = u_0^2 - v_0^2, \qquad y = 2u_0v_0. \tag{6.5}$$

The path of steepest descent through w_0 is given by the equation

$$u = u_0 + \frac{(v - v_0)(v + 2v_0)}{3\left[u_0 + \sqrt{\frac{1}{3}(v^2 + 2v_0v + 3u_0^2)}\right]}, \qquad -\infty < v < \infty. \tag{6.6}$$

Examples for $r = 5$ and a few θ-values are shown in figure 3. The saddle points are located on the circle with radius $\sqrt{r}$ and are indicated by small dots.

The saddle point on the positive real axis corresponds with the case $\theta = 0$ and the two saddles on the imaginary axis with the case $\theta = \pi$. This is out of the range of present interest, but it is instructive to see that the contour may split up and run through both saddle points $\pm w_0$.

In our numerical algorithm we use numerical quadrature for the integral (6.1), and we use a contour through the saddle point w_0.

Integrating with respect to $\tau = u - u_0$ (and writing $\sigma = v - v_0$) we obtain

$$\mathrm{Ai}(z) = \frac{\mathrm{e}^{-\zeta}}{2\pi\mathrm{i}}\int_{-\infty}^{\infty} \mathrm{e}^{\psi_r(\sigma,\tau)}\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\tau} + \mathrm{i}\right)\mathrm{d}\tau, \tag{6.7}$$

where $\zeta = \frac{2}{3}z^{3/2}$, and

$$\sigma = \frac{\tau(\tau + 3v_0)}{3[u_0 + \sqrt{(1/3)(\tau^2 + 4v_0\tau + 3r)}]}, \qquad -\infty < \tau < \infty, \tag{6.8}$$

$$\psi_r(\sigma, \tau) = \Re\left[\phi(w) - \phi(w_0)\right] = u_0\left(\sigma^2 - \tau^2\right) - 2v_0\sigma\tau + \frac{1}{3}\sigma^3 - \sigma\tau^2. \tag{6.9}$$

Further details can be found in [10].

7. Concluding remarks

1. The mathematical software for special functions is not at all complete when one needs function values for the case of large and complex parameters. Examples are Airy functions, Bessel functions with complex order and parabolic cylinder functions.

2. We have come to the conclusion that quadrature methods are of great importance in the evaluation of special functions, in particular when parameters are large and complex. Methods based on asymptotic analysis can be used to select suitable integral representations, and to separate dominant terms as factors in front of the integrals.

3. The trapezoidal rule is a flexible tool for evaluating a large class of special functions. For an important class of integrals this rule is very efficient and can produce very accurate results.

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