Special Functions and Computer Algebra

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Contents

Asymptotics, Special Functions

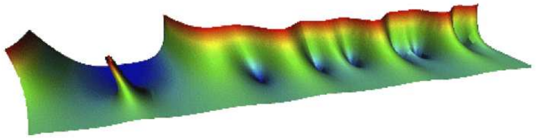
- Book: Roderick Wong, *Asymptotic Approximations of Integrals*, SIAM, 2001.
- Book: Gil et al. *Numerical Methods for Special Functions*, SIAM, 2007.
- Software survey: Lozier and Olver, Numerical evaluation of special functions (1994). Updates are available at http://math.nist.gov/mcsd/Reports/2001/nesf/
- Other books: Baker (1992), Moshier (1989), Thompson (1997), Zhang & Jin (1996), Numerical Recipes.
- Software: many collections on the web.

Asymptotics, Special Functions

The NIST Handbook of Mathematical Functions.
The revision of Abramowitz & Stegun, *Handbook of Mathematical Functions*.

Free available at http://dlmf.nist.gov/
Book edition: CUP, June 2010.

Asymptotics, Special Functions



NIST Digital Library of Mathematical Functions

companion to the NIST Handbook of Mathematical Functions

Project News

2010-05-11 *Handbook published and DLMF goes public*
2010-05-06 *Firefox 3.6 slow on Windows*

- *More news*

Asymptotics, Special Functions

To compute: generalized forms? (Meijer, Fox, ...). For example, the generalized hypergeometric function:

$$ {}_pF_q\left(\begin{matrix} a_1, \cdots, a_p \\ b_1, \cdots, b_q \end{matrix}; z\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{z^n}{n!}, $$

where $p \le q+1$ and $(a)_n$ is the Pochhammer symbol, also called the shifted factorial, defined by

$$ (a)_0 = 1, \quad (a)_n = a(a+1)\cdots(a+n-1)\ (n \ge 1). $$

Use special cases and several methods: power series, asymptotic series, and in between?

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Some simple experiences

- How to compute this integral ?
- Another integral
- Exponential integral: $\mathrm{Ei}(x)$ or $\mathrm{Ei}(z)$?
- Take a special case
- Scaling
- Example: Confluent hypergeometric function

How to compute this integral ?

Consider

$$F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}}\,dt.$$

- Maple 13, for $\lambda = 10$, gives

$$F(10) = -.1837516481 + .5305342893i.$$

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- With Digits = 40, the answer is

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$$0.5305342892550606876095028928250448740020i.$$

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$$0.5305342892550606876095028928250448740020i.$$

- So, the first answer seems to be correct in all shown digits.

How to compute this integral ?

Take another integral, which is almost the same:

$$F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}}\,dt \implies G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda t}\,dt.$$

- Maple 13, with *evalf(Int...*, gives
  $G(10) = -1.249000903 \times 10^{-16}$

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- The correct answer is $G(10) = 0.6593662989 \times 10^{-43}$.

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- The correct answer is $G(10) = 0.6593662989 \times 10^{-43}$.
- Maple 13, with procedure *int*, gives $G(10) = e^{-100}\sqrt{\pi}$.

How to compute this integral ?

The message is: one should have some feeling about the computed result.

Otherwise a completely incorrect answer can be accepted.

Mathematica 7 is more reliable here, and gives a warning with answer $0. \times 10^{-16} + 0. \times 10^{-17} i$.

Another integral

Consider

$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}.$$

Mathematica 7 gives the correct expression of $F(u)$ in terms of sine and cosine integrals, and gives the correct numerical value

$$F(2) = -0.934349\ldots - 0.70922\ldots i.$$

$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}$$

In earlier days Mathematica 4.1 gave for $u = 2$ in terms of the Meijer G-function:

$$F(2) = \pi G_{2,3}^{2,1}\left(\begin{matrix} 0, \ \frac{1}{2} \\ 0, 0, \frac{1}{2} \end{matrix} ; \ 2 - 2i \right).$$

Mathematica 4.1 evaluated the false answer: $F(2) = -0.547745 - 0.532287i$.

On the other hand, Mathematica 4.1 produced

$$F(u) = e^{iu-u}\Gamma(0, iu - u),$$

(which is also false) in terms of the incomplete gamma function.

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$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}$$

This gives the wrong answer
$F(2) = -0.16114 - 0.355355i$.

So, we had three numerical results:

$$F_1 = -0.934349 - 0.70922i,$$

$$F_2 = -0.547745 - 0.532287i,$$

$$F_3 = -0.16114 - 0.355355i.$$

Observe that $F_2 = (F_1 + F_3)/2$.

F_1 is correct.

$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}$$

Maple 13 gives

$$F(u) = e^{iu-u}\mathrm{Ei}(1, iu - u).$$

Here $\mathrm{Ei}(z)$ is an exponential integral, which can be written as the Mathematica 4.1 false answer $e^{iu-u}\Gamma(0, iu - u)$.
When we use in Maple $assume(u > 0)$, then we obtain

$$F(u) = e^{iu-u}\mathrm{Ei}(1, iu - u) + 2\pi i\, e^{iu-u},$$

which is, in some sense, correct.

$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}$$

Also, Maple 13 gives for the given value $u = 2$

$$F(2) = e^{2i-2}\mathrm{Ei}(1, 2i-2) + 2\pi i\, e^{2i-2},$$

giving $F(2) = -.9343493872 - .7092195102i$, and this is the correct answer.

Maple 13 gives the correct numerical value for $F(-2)$.

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Exponential integral: $\mathrm{Ei}(x)$, $\mathrm{Ei}(z)$

The exponential integrals are defined by

$$E_1(z) = \int_1^\infty \frac{e^{-zt}}{t}\,dt, \qquad E_n(z) = \int_1^\infty \frac{e^{-zt}}{t^n}\,dt, \qquad |\mathrm{ph}\, z| < \pi,$$

$$\mathrm{Ei}(x) = -\fint_{-x}^{\infty} \frac{e^{-t}}{t}\,dt = \fint_{-\infty}^{x} \frac{e^{t}}{t}\,dt, \qquad x > 0,$$

(principal value integrals)

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty} \frac{e^{-t}}{t}\,dt = -E_1(-x), \qquad x < 0.$$

Exponential integral: $\mathrm{Ei}(x)$, $\mathrm{Ei}(z)$

Earlier Maple required real x in $\mathrm{Ei}(x)$, as is in agreement with this definition.

Unfortunately, Maple 13 uses

$$\mathrm{Ei}(a,z) = z^{a-1}\Gamma(1-a,z) = \int_z^\infty \frac{e^{-zt}}{t^a}\,dt, \qquad \Re z > 0.$$

It should use the notation $E_a(z)$ for genearl complex a and $|\mathrm{ph}\, z| < \pi$.

Exponential integral: $\mathrm{Ei}(x)$, $\mathrm{Ei}(z)$

Mathematica 7 (and earlier) accepts complex z in $\mathrm{Ei}(z)$.

However, *The Mathematica Book* (4th Ed., p. 765) defines $\mathrm{Ei}(z)$ only for $z > 0$ by using a principal value integral.

This is confusing.

Take a special case

Parabolic cylinder functions are special cases of the ${}_1F_1$ functions, Kummer functions or Whittaker functions.
The Mathematica Book (4th Ed., p. 765) advises to use the Whittaker function

$$U(a,z) = 2^{-a/2} z^{-1/2} W_{-a/2,-1/4}\left(\tfrac{1}{2}z^2\right),$$

but this is useless when $z < 0$.

Mathematica 7 gives now the function $D_\nu(z)$, which seems to perform quite well.

Take a special case

Mathematic 7 evaluates

ParabolicCylinderD[-300.14, 300.15]

in a split second: $6.83322814925 * 10^{-10526}$, the correct answer being $6.833323122 * 10^{-10526}$.

Maple 13 comes with the answer $7.05770276159934 * 10^{9807}$, after 5 seconds.

Scaling

The function $\Gamma^*(z)$ defined by

$$\Gamma(z) = \sqrt{2\pi} z^{z-1/2} e^{-z} \Gamma^*(z),$$

$$\Gamma^*(z) \sim 1 + \frac{1}{12z} + \frac{1}{288z^2} + \ldots, \qquad z \to \infty,$$

can be computed within machine precision for almost all complex z. The precision in the gamma function itself follows from the evaluation of the elementary function

$$\sqrt{2\pi} z^{z-1/2} e^{-z}.$$

To avoid underflow and overflow, and to control accuracy, it is very important to have scaled functions like $\Gamma^*(z)$ available.

The same holds for Bessel functions, parabolic cylinder functions, and so on.

The scaled Airy function $\widetilde{\mathrm{Ai}}(z)$ defined by

$$\mathrm{Ai}(z) = e^{-\frac{2}{3}z^{3/2}}\,\widetilde{\mathrm{Ai}}(z)$$

can be computed very accurate for complex z (not close to zeros of $\mathrm{Ai}(z)$).

The scaling factor $e^{-\frac{2}{3}z^{3/2}}$ completely determines the accuracy if z is large and complex.

Again, scaled functions are very useful to avoid underflow and overflow, and to control accuracy.

Kummer U–function

The standard solution of Kummer's equation that is singular at the origin can be written in the form

$$U(a,c,z) = \frac{\pi}{\sin \pi c}\left(\frac{{}_1F_1(a;c;z)}{\Gamma(1+a-c)\Gamma(c)} - z^{1-c}\frac{{}_1F_1(1+a-c;2-c;z)}{\Gamma(a)\Gamma(2-c)}\right).$$

Also, for $\Re a > 0, \Re z > 0$,

$$U(a,c,z) = \frac{1}{\Gamma(a)}\int_0^\infty e^{-zt}t^{a-1}(1+t)^{c-a-1}\,dt.$$

Kummer $U-$function

For small z the series of the ${}_1F_1-$functions can be used for computations. For large z the ${}_1F_1-$functions become exponentially large, while the $U-$function becomes $\mathcal{O}(z^{-a})$.

Also, for integer values of c, problems arise when we use the representation in terms of the ${}_1F_1-$functions.

A careful analysis is needed to avoid numerical cancellations.

Kummer U−function

We can write

$$U(a,c,z) = \sum_{k=0}^{\infty} u_k z^k,$$

$$u_0 = \frac{\pi}{\sin \pi c} \frac{1}{\Gamma(1+a-c)\Gamma(c)} = \frac{\Gamma(1-c)}{\Gamma(1+a-c)},$$

$$u_1 = \frac{\pi}{\sin \pi c} \left[\frac{a}{\Gamma(1+c)\Gamma(1+a-c)} - \frac{z^{-c}}{\Gamma(a)\Gamma(2-c)} \right].$$

For small values of c the coefficient u_1 is difficult to compute.

Gauss hypergeometric functions

For many parameter values a, b, c the Gauss function is an elementary function.

For example:

$$ {}_2F_1\left(\begin{matrix} a, \; 1-a \\ \frac{1}{2} \end{matrix}; \sin^2 z\right) = \frac{\cos((2a-1)z)}{\cos z}, $$

$$ {}_2F_1\left(\begin{matrix} a, \; 1-a \\ \frac{3}{2} \end{matrix}; \sin^2 z\right) = \frac{\sin((2a-1)z)}{(2a-1)\sin z}. $$

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Gauss hypergeometric functions

Maple 13 gives the second form, not the first one (although it gives ${}_2F_1(a,1-a;1/2;-z^2)$).

Mathematica 7 gives both forms.

When ${}_2F_1(a,b;c;z)$ is a simple function, all ${}_2F_1(a+k,b+\ell;c+m;z)$ are simple for integer k,ℓ,m.

This follows from the recursion relations.

Maple 13 and Mathematica 7 don't give ${}_2F_1(a+1,1-a;1/2;z)$; Mathematica gives this with *FunctionExpand*.

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Asymptotic expansions

Maple 13 LaTeX output: via *asympt*

$$\Gamma(z) \sim \left(\sqrt{2}\sqrt{\pi}\sqrt{z^{-1}} + \frac{1}{12}\sqrt{2}\sqrt{\pi}\left(z^{-1}\right)^{3/2} + \frac{1}{288}\sqrt{2}\sqrt{\pi}\left(z^{-1}\right)^{5/2} - \frac{139}{51840}\sqrt{2}\sqrt{\pi}\left(z^{-1}\right)^{7/2} + \mathcal{O}\left(\left(z^{-1}\right)^{9/2}\right)\right)\left(\left(z^{-1}\right)^{z}\right)^{-1}\left(\mathrm{e}^{z}\right)^{-1}$$

or more terms when requested.

Asymptotic expansions

We like to see

$$\Gamma(z) \sim \sqrt{2\pi} e^{-z} z^{z-\frac{1}{2}} \left(1 + \frac{1}{12} z^{-1} + \frac{1}{288} z^{-2} - \frac{139}{51840} z^{-3} + \mathcal{O}\left(z^{-4}\right)\right),$$

or more terms when requested.

In this form it is easier to see the structure and to collect the coefficients.

The same happens with other well-known special functions (for example, the complementary error function, incomplete gamma functions, ...).

Asymptotic expansions

When we ask the large z asymptotic expansion of $\Gamma(z+a)$ we obtain in Maple13:
Error, (in asympt) unable to compute series

The same happens when we ask the large z asymptotic expansion of $\Gamma(z+a)/\Gamma(z+b)$, which reads

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} \sim z^{a-b}\left(1+\frac{(a-b)(a+b-1)}{2z}+\mathcal{O}\left(z^{-2}\right)\right).$$

Mathematica 7 gives the asymptotic expansion of $\Gamma(z+a)$ (although not in a nice form), and the expansion of $\Gamma(z+a)/\Gamma(z+b)$ in a better form.

Asymptotic expansions

How to obtain?

The first form is the Laplace transform

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt,$$

with, say, f analytic at the origin and for $t > 0$; also, $f(t) = \mathcal{O}(\exp(\alpha t))$ for large t.

In practical problems, first a transformation into this standard form is needed.

Asymptotic expansions

Then,

$$f(t) = \sum_{n=0}^{\infty} a_n t^n \quad \text{(a local expansion)}$$

gives (Watson's lemma)

$$F(s) \sim \sum_{n=0}^{\infty} a_n \frac{n!}{s^{n+1}}, \qquad s \to \infty.$$

Asymptotic expansions

A simple example:

$$F(s) = \int_0^\infty e^{-s \sinh u} \frac{du}{1+u}.$$

A transformation is needed to bring this into a Laplace integral. Write

$$t = \sinh u, \quad \text{or} \quad u = \operatorname{arcsinh} t.$$

Then

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt, \quad f(t) = \frac{1}{1+u} \frac{du}{dt}.$$

Asymptotic expansions

We need to expand $f(t) = \sum_{n=0}^{\infty} a_n t^n$.

Because $dt/du = \cosh u = \sqrt{1+t^2}$, we have

$$f(t) = \frac{1}{1+u}\frac{du}{dt} = \frac{1}{1+\operatorname{arcsinh} t}\frac{1}{\sqrt{1+t^2}},$$

and it is not difficult to obtain the coefficients a_n and the asymptotic expansion.

Asymptotic expansions

This example is simple because the inversion of the transformation $u = \sinh t$ is explicitly known, and so is $f(t)$, as a function of t.

In the following example

$$F(s) = \int_0^\infty e^{-s\,\phi(u)}\,\frac{du}{1+u}, \qquad \phi(u) = u\sqrt{1+u^3},$$

the inverse of the substitution $t = \phi(u)$ is properly defined for $u \geq 0$, but this inverse is not explicitly known.

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Asymptotic expansions

So, the function $f(t)$ in

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt, \qquad f(t) = \frac{1}{1+u} \frac{du}{dt},$$

cannot straightforwardly be expanded in powers of t.

We need extra computer algebra to do this.

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Asymptotic expansions

First the relation $t = u\sqrt{1+u^3}$ has to be inverted in the form

$$u = \sum_{n=1}^{\infty} b_n t^n, \qquad \frac{du}{dt} = \sum_{n=1}^{\infty} n b_n t^{n-1},$$

from which the expansion of $f(t)$ easily follows.

Manipulating power series, inverting relations, and so on, are needed here, and are easy to perform with the help of computer algebra.

Asymptotic expansions

Similar methods can be used for the integral

$$F(\omega) = \int_{-\infty}^{\infty} e^{-\omega t^2} f(t)\, dt, \quad \text{as} \quad \omega \to \infty.$$

The point $t = 0$ is the dominant point for this integral. The local expansion $f(t) = \sum_{n=0}^{\infty} c_n t^n$ gives

$$F(\omega) \sim \sum_{n=0}^{\infty} c_{2n} \int_{-\infty}^{\infty} e^{-\omega t^2} t^{2n}\, dt,$$

that is,

$$F(\omega) \sim \sum_{n=0}^{\infty} c_{2n}\, \Gamma(n + \tfrac{1}{2}) \omega^{-n-\frac{1}{2}}, \quad \text{as} \quad \omega \to \infty.$$

Asymptotic expansions

Integrals of this type arise in the saddle point method, after transformation to this standard form.

The transformation may be defined properly, but it may not have an explicit inverse.

This occurs in the following case

$$\Gamma(z) = \int_0^\infty v^{z-1} e^{-v}\, dv.$$

A simple transformation $v = z(1+u)$ gives

$$\Gamma(z) = z^z e^{-z} \int_{-1}^\infty e^{-z\phi(u)} \frac{du}{u+1}, \qquad \phi(u) = u - \ln(1+u).$$

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Asymptotic expansions

The main contribution comes from $u = 0$, where $\phi'(u) = u/(1+u)$ vanishes ($u = 0$ is called a *saddle point*).
For small u we have

$$\phi(u) = \tfrac{1}{2}u^2 - \tfrac{1}{3}u^3 + \ldots,$$

and we transform

$$\phi(u) = \tfrac{1}{2}t^2, \quad \mathrm{sign(u)} = \mathrm{sign(t)}.$$

This gives

$$\Gamma(z) = z^z e^{-z} \int_{-\infty}^{\infty} e^{-\frac{1}{2}zt^2} f(t)\, dt, \quad f(t) = \frac{1}{1+u}\frac{du}{dt}.$$

Asymptotic expansions

From the mapping we can obtain the inverse in the form

$$u = \sum_{n=1}^{\infty} b_n t^n,$$

and hence the expansion

$$f(t) = \sum_{n=0}^{\infty} c_n t^n.$$

In a similar way we can obtain the asymptotic expansion of $\Gamma(z+a)$.

Asymptotic expansions

From linear forms

$$F(\omega) = \int_0^\infty e^{-\omega t} f(t)\, dt$$

and quadratic forms

$$F(\omega) = \int_{-\infty}^\infty e^{-\omega t^2} f(t)\, dt,$$

with $\omega \to \infty$, we can generalize further, but these are the basic forms.
Other (more complicated) inversion problems arise in so-called *uniform asymptotic expansions*.

Asymptotic expansions

In uniform expansions expansions two-point Taylor expansions of the type

$$f(t) = \sum_{n=0}^{\infty} (a_n + b_n t)(t^2 - t_0^2)^n$$

are needed. Typically, $\pm t_0$ are two relevant saddle points.

The coefficients can be expressed in terms of the derivatives of f at $\pm t_0$.
But because f is usually obtained from a transformation of which the inverse is not explicitly available (or difficult to handle), the computation of the coefficients is quite complicated.

Without computer algebra even impossible, sometimes.

Uniform asymptotic expansions

A simple uniform expansion can be derived of the generalized exponential integral

$$E_n(x) = \int_1^\infty e^{-xu} \frac{du}{u^n}$$

for the case that $x + n \to +\infty$.

Write $n = \nu x$ and obtain

$$E_n(x) = \int_1^\infty e^{-x\phi(u)}\, du, \qquad \phi(u) = u + \nu \ln u.$$

Uniform asymptotic expansions

Because $\phi'(u) = 1 + \nu/u > 0$ we can substitute $t = \phi(u) - 1$ and obtain

$$E_n(x) = e^{-x} \int_0^\infty e^{-xt} f(t)\, dt, \qquad f(t) = \frac{du}{dt} = \frac{1}{\phi'(u)}.$$

An inversion procedure gives the required expansion

$$f(t) = \sum_{m=0}^{\infty} c_m(\nu) t^m,$$

from which the asymptotic expansion follows.

Uniform asymptotic expansions

The incomplete gamma function $Q(a, z)$ defined by

$$Q(a, x) = \frac{1}{\Gamma(a)} \int_x^\infty t^{a-1} e^{-t} \, dt$$

can be written in terms of the error function:

$$Q(a, x) = \tfrac{1}{2} \operatorname{erfc}(\eta\sqrt{a/2}) + R_a(\eta),$$

where

$$R_a(\eta) \sim \frac{e^{-\frac{1}{2}a\eta^2}}{\sqrt{2\pi a}} \sum_{n=0}^{\infty} \frac{C_n(\eta)}{a^n}, \qquad a \to \infty,$$

uniformly with respect to $x \geq 0$.

Uniform asymptotic expansions

Here,

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\, dt,$$

and

$$\tfrac{1}{2}\eta^2 = \lambda - 1 - \ln\lambda, \qquad \lambda = \frac{x}{a}.$$

We have

$$C_0(\eta) = \frac{1}{\lambda - 1} - \frac{1}{\eta},$$

and

$$C_1(\eta) = \frac{1}{\eta^3} - \frac{1}{(\lambda-1)^3} - \frac{1}{(\lambda-1)^2} - \frac{1}{12(\lambda-1)}.$$

Singularities appear when $\lambda = 1$ (and $\eta = 0$), but all coefficients are analytic at these points.

Recursions to compute SF's

Many special functions coming from the family of hypergeometric functions satisfy three-term recurrence relations of the form

$$A_n y_{n-1} + B_n y_n + C_n y_{n+1} = 0.$$

When we give two consecutive values, say the pair $\{y_0, y_1\}$, other values y_n can be generated by using the recursion.

Recursions to compute SF's

Examples are

- Bessel functions,
- Legendre functions,
- Incomplete gamma and beta functions,
- Gauss hypergeometric functions,
- Confluent (or Kummer) hypergeometric functions.

Recursions to compute SF's

As is usual in numerical computations: stability of computations is an important aspect here. Choosing the direction of computation (that is, choosing forward or backward recursion) is an essential option.

For example, the Bessel function $J_n(x)$ should not be computed with starting values $\{J_0(x), J_1(x)\}$. There are efficient algorithms, based on backward recursion, to compute $J_n(x)$.

Recursions to compute SF's

More generally: let $\{f_n, g_n\}$ be a solution pair of

$$A_n y_{n-1} + B_n y_n + C_n y_{n+1} = 0$$

with the property

$$\lim_{n \to +\infty} \frac{f_n}{g_n} = 0,$$

then f_n is called a minimal solution and should not be computed in the forward direction.

The computation of g_n, a dominant solution, is stable in the forward direction.

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Quadrature of integrals

A simple example is:

$$G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda t}\,dt = e^{-\lambda^2}\int_{-\infty}^{\infty} e^{-s^2}\,ds.$$

This makes sense, because

- The new integral is real, without oscillations
- The dominant term $e^{-\lambda^2}$ is in front of the new integral

Trapezoidal rule

$$\int_a^b f(t)\,dt = \frac{1}{2}h[f(a)+f(b)]+h\sum_{j=1}^{n-1} f\,(h\,j)+R_n, \qquad h=\frac{b-a}{n}.$$

- Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.

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Trapezoidal rule

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- Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.
- Error term, for some $\xi \in (a,b)$:

$$R_n = -\frac{n\,h^3}{12}\,f''(\xi).$$

Trapezoidal rule

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- Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.
- Error term, for some $\xi \in (a,b)$:

$$R_n = -\frac{n\,h^3}{12}\,f''(\xi).$$

- Adaptive algorithm: use previous function values $(h \longrightarrow h/2)$.

Example: fast convergence

Example: the $J-$Bessel function ($h = \pi/n$, $x = 5$)

$$\pi\, J_0(x) = \int_0^\pi \cos(x \sin t)\, dt = h + h \sum_{j=1}^{n-1} \cos\left[x \sin(h\, j)\right] + R_n,$$

n	R_n
4	$-.12\ 10^{-0}$
8	$-.48\ 10^{-6}$
16	$-.11\ 10^{-21}$
32	$-.13\ 10^{-62}$
64	$-.13\ 10^{-163}$
128	$-.53\ 10^{-404}$

The remainder can be very small

This is much better than the estimate of R_n.
Explanation: periodicity and smoothness.

In fact we have

Theorem

If f is periodic and has a continuous k^{th} derivative, and if the integral is taken over a period, then

$$|R_n| \leq \frac{\text{constant}}{n^k}.$$

Bessel function: we can take any k and R_n may be exponentially small for large n.

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The trapezoidal rule on $\mathbb{R}$

For integrals over $\mathbb{R}$ the trapezoidal rule may again be very efficient and accurate.
Consider

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

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

We use this for functions analytic in the strip:

$$G_a = \{z = x + iy \quad | \quad x \in \mathbb{R},\ -a < y < a\}.$$

A class of analytic functions

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

$$\lim_{x\to\pm\infty} f(x+iy) = 0$$

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

$$M_{\pm a}(f) = \int_{-\infty}^{\infty} |f(x \pm ia)|\, dx =$$

$$\lim_{b\uparrow a} \int_{-\infty}^{\infty} |f(x \pm ib)|\, dx < \infty.$$

The error is exponentially small

Theorem

Let $f \in H_a$ for some $a > 0$, and f even. Then

$$|R_d(h)| \leq \frac{e^{-\pi a/h}}{\sinh(\pi a/h)} M_a(f),$$

for any y with $0 < y < a$.

Proof

The proof is based on residue calculus. See Gil et al. (2007).

Example: $K-$Bessel function

Consider the modified Bessel function

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

We have, with $d = 0$,

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

Example: $K-$Bessel function

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

h	j_0	$R_0(h)$
1	2	$-.18\ 10^{-1}$
$1/2$	5	$-.24\ 10^{-6}$
$1/4$	12	$-.65\ 10^{-15}$
$1/8$	29	$-.44\ 10^{-32}$
$1/16$	67	$-.19\ 10^{-66}$
$1/32$	156	$-.55\ 10^{-136}$
$1/64$	355	$-.17\ 10^{-272}$

Fast convergent; easy to program

- We see in this example that, halving the value of h gives a doubling of the number of significant digits.
- 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.

CWI

Other numerical methods

For the *basic methods* discussed earlier see Gil et al. (2007). Other topics discussed are

- Chebyshev expansions, Continued fractions
- Zeros of special functions
- Uniform asymptotic expansions
- Padé approximants, Sequence transformations
- Best rational approximation
- Inversion of cumulative distribution functions
- The Euler summation formula
- Numerical inversion of Laplace transforms

Concluding remarks

Last Friday I received the following email:

```
Hi, I’m a student from China. Recently, I’m
doing some research on the special function:
Meijer G function. I want to ask you something
about: How to numerical computing the function.

I mean that I want to write a program to
compute the function, although, Maple and
Mathematica can compute it. Could you give
me some idea or material about it?
```

My first reaction was: poor student.

Concluding remarks

For me computer algebra is important because of

- Obtaining coefficients and saddle point contours in asymptotic expansions.
- Checking formulas and relations in new software for special functions.
- Checking the performance of new software for special functions.
- Maple and Mathematica are great tools for doing this and for other applications.
- But I'm careful, and don't trust or accept all answers.