Numerical Aspects of Special Functions

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- The procurement will be competitive among qualified mathematics publishers.

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- In addition to the print edition, the DLMF will be distributed free from a public Web site at NIST. The Web address is http://dlmf.nist.gov. A sample chapter on Airy functions has existed on this Web site since the beginning of the project.

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- More than 50 individuals are contributing to the project as paid authors and validators. The staff at NIST consists of another dozen or so people.

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- A complete survey of the available software: Lozier & Olver (1994); last update: December 2000.
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- Books with software: Baker, Moshier, Numerical Recipes, Thompson, Wong & Guo, Zhang & Jin.

A book on numerics of special functions

The topics mentioned in this lecture, and several other topics, will be discussed extensively, with examples of software, in a new book with the title

Numerical Methods for Special Functions.

Written together with my co-authors Amparo Gil and Javier Segura (Santander, Spain).

We have just submitted the first version for review.

To be published by SIAM.

A book on numerics of special functions

As the basic methods for computing special functions we consider

- Power series: convergent, asymptotic
- Chebyshev series
- Recurrence relations and continued fractions
- Quadrature methods

A book on numerics of special functions

Other important methods and aspects are

- Continued fractions
- Computation of the zeros of special functions
- Padé approximations
- Sequence transformations
- Best rational approximations

A book on numerics of special functions

Other topics are

- The Euler summation formula
- Numerical solution of ODEs: Taylor expansion method
- Uniform asymptotic expansions
- Asymptotic inversion of distribution functions
- Symmetric elliptic integrals
- Numerical inversion of Laplace transforms
- Approximations of Stirling Numbers
- Oscillatory integrals

A book on numerics of special functions

In the software section we discuss mainly the G-S-T Fortran codes published earlier. Routines can be downloaded from http://personales.unican.es/segurajj/book/software.html

- Airy and Scorer functions of complex arguments and their derivatives.
- Legendre functions of integer and half-odd degrees; toroidal harmonics.
- Modified Bessel functions of integer and half integer orders.
- Modified Bessel functions of purely imaginary orders.
- Parabolic cylinder functions.
- Zeros of the Bessel function $J_\nu(x)$.

Recursion relations

To compute

- Bessel functions
- Legendre functions
- Confluent hypergeometric functions (Kummer, Whittaker, Coulomb)
- Parabolic cylinder functions
- Gauss hypergeometric functions
- Incomplete gamma and beta functions
- Orthogonal polynomials

recursion relations are important and frequently used.

Recursion relations

The recursion relations are of the form

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \quad n = 1, 2, 3, \ldots$$

When there are two linearly independent solutions $\boldsymbol{f_n}$ and $\boldsymbol{g_n}$, such that

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

the computation of the minimal solution

$$f_n, \quad n = 2, 3, 4, \ldots$$

from $\boldsymbol{f_0}$ and $\boldsymbol{f_1}$ (forward recursion) is usually very unstable. The solution $\boldsymbol{g_n}$ is called a dominant solution.

Recursion relations

For example, the functions

$$f_n(x) = e^x - 1 - x - \cdots - \frac{x^{n-1}}{(n-1)!}, \quad f_0(x) = e^x, \quad f_1(x) = e^x - 1,$$

satisfy the recursion relation

$$y_{n+1} - \left(1 + \frac{x}{n}\right) y_n + \frac{x}{n} y_{n-1} = 0, \quad n = 1, 2, 3, \ldots$$

Computing $\boldsymbol{f_n(1)}$ with Maple, standard 10 Digits, we see that

$$f_{13}(x) = -0.340710500 \times 10^{-9},$$

a negative number.

Recursion relations

The function

$$g_n(x) = e^x - f_n(x) = 1 + x + \cdots + \frac{x^{n-1}}{(n-1)!},$$

is for $x > 0$ a dominant solution of the recursion.

It can be computed in a stable way with starting values

$$g_0(x) = 0, \quad g_1(x) = 1.$$

Recursion relations

The recursion for the functions $f_n(x)$ follows from the simpler (inhomogeneous) recursion

$$y_{n+1} = y_n - \frac{x^n}{n!}.$$

Use this in backward direction with false starting value $f_{21}(1) = 0$. Then

$$f_{13}(1) = 1.7287667139 \times 10^{-10} \ldots,$$

which is correct in all shown digits.

Backward recursion for a minimal solution with false starting values is the basis for the Miller algorithm.

Parabolic cylinder functions

PCFs are solutions of the differential equation

$$w'' - \left(\frac{1}{4}x^2 + a\right) w = 0.$$

Special cases:

- Hermite polynomials $2^{-n/2} e^{-x^2/4} H_n(x/\sqrt{2})$ when $a = -n - \frac{1}{2}$, $n = 0, 1, 2, \ldots$.
- complementary error function $\sqrt{\pi/2} e^{x^2/4} \mathrm{erfc}(x/\sqrt{2})$ when $a = \frac{1}{2}$.
- PCFs are special cases of Kummer functions (confluent hypergeometric functions).

Parabolic cylinder functions

Two linearly independent solutions of the differential equations are denoted by $U(a,x)$ and $V(a,x)$.

Another notation is $D_a(x) = U(-a-\frac{1}{2},x)$.

Scaling is very important to prevent underflow and overflow (and to extend the domains for computation).

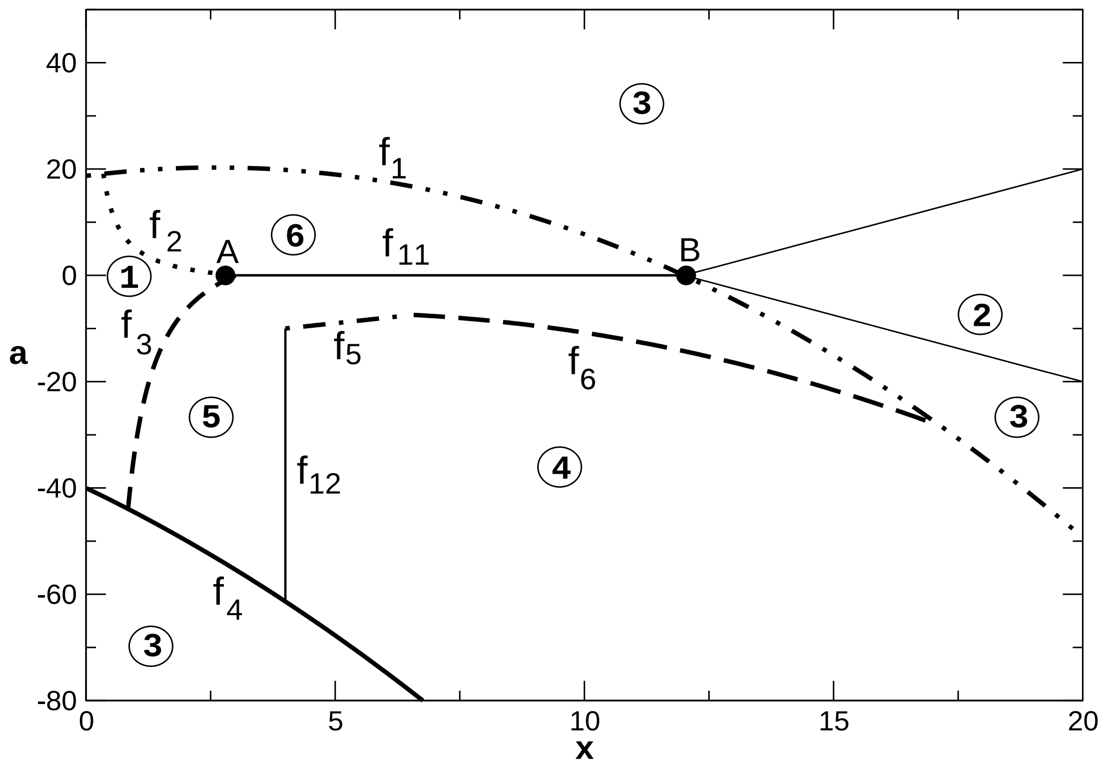
When $a \ge 0$ the computation is not too difficult.

When $a < 0$ and $\frac{1}{4}x^2 < -a$, oscillations occur.

Large parameters a and x, with $\frac{1}{4}x^2 \sim -a$, are especially difficult to handle.

Parabolic cylinder functions

The regions in the (a, x)-plane where different methods of computation for PCFs are considered. Only for $x \geq 0$; for negative x connection formulas are used.



Parabolic cylinder functions

Maclaurin series

In region 1 (small a and x) we use Maclaurin series

$$y_1(a,x) = \left\{1 + a\frac{x^2}{2!} + (a^2+1/2)\frac{x^4}{4!} + \ldots\right\},$$

$$y_2(a,x) = \left\{x + a\frac{x^3}{3!} + (a^2+3/2)\frac{x^5}{5!} + \ldots\right\}.$$

Recursion relations for the coefficients are used.

y_1 and y_2 are solutions of the differential equation, but do not constitute a *numerically satisfactory pair of solutions* for large values of x.

Parabolic cylinder functions

y_1 and y_2 are used in

$$U(a,x) = U(a,0)y_1(a,x) + U'(a,0)y_2(a,x),$$

$$V(a,x) = V(a,0)y_1(a,x) + V'(a,0)y_2(a,x),$$

with

$$U(a,0) = \frac{\sqrt{\pi}}{2^{\frac{a}{2}+\frac{1}{4}}\Gamma(\frac{3}{4}+\frac{1}{2}a)}, \quad U'(a,0) = -\frac{\sqrt{\pi}}{2^{\frac{a}{2}-\frac{1}{4}}\Gamma(\frac{1}{4}+\frac{1}{2}a)},$$

$$V(a,0) = \frac{2^{\frac{a}{2}+\frac{1}{4}}\sin\pi(\frac{3}{4}-\frac{1}{2}a)}{\Gamma(\frac{3}{4}-\frac{1}{2}a)}, \quad V'(a,0) = \frac{2^{\frac{a}{2}+\frac{3}{4}}\sin\pi(\frac{1}{4}-\frac{1}{2}a)}{\Gamma(\frac{1}{4}-\frac{1}{2}a)}.$$

Parabolic cylinder functions

In other regions we use

- Quadrature
- Recursions with computed starting values
- Poincaré asymptotic expansions (in powers of x^{-1})
- Uniform asymptotic expansions in terms of elementary functions
- Uniform asymptotic expansions in terms of Airy functions

Parabolic cylinder functions

Quadrature

For quadrature we transform some standard integrals into integrals that can easily be evaluated by using the *trapezoidal rule*.

It is well known that integrals of the type

$$\int_{-\infty}^{\infty} e^{-zt^2} f(t)\, dt, \qquad (*)$$

with f analytic inside a strip $|\Im t| < a$, for some $a > 0$, are excellent starting points for the trapezoidal rule.

Parabolic cylinder functions

In many cases we transform finite integrals, say of the form

$$\int_{-1}^{1} f(t)\,dt,$$

into an integral of the form $(*)$ by using the error function:

$$t = \operatorname{erf} s = \frac{2}{\sqrt{\pi}} \int_0^s e^{-u^2}\,du,$$

and the integral becomes

$$\int_{-1}^{1} f(t)\,dt = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-s^2} f(\operatorname{erf}(s))\,ds.$$

Using special functions

Special functions play an important role in

- The solution of problems in mathematical physics, engineering, statistics, and so on.
- As kernels in integral transforms.
- ...
- ...

Using special functions

The non-central chi-squared distributions

The definition are for positive x, y, μ:

$$P_\mu(x,y) = e^{-x}\sum_{n=0}^{\infty}\frac{x^n}{n!}P(\mu+n,y), \quad Q_\mu(x,y) = e^{-x}\sum_{n=0}^{\infty}\frac{x^n}{n!}Q(\mu+n,y),$$

where P and Q are the incomplete gamma functions:

$$P(a,x) = \frac{1}{\Gamma(a)}\int_0^x t^{a-1}e^{-t}\,dt, \quad Q(a,x) = \frac{1}{\Gamma(a)}\int_x^\infty t^{a-1}e^{-t}\,dt.$$

$$P_\mu(x,y) + Q_\mu(x,y) = 1.$$

Using special functions

The non-central chi-squared distributions

Recursion relations are:

$$P_{\mu+1}(x,y) = P_\mu(x,y) - \left(\frac{y}{x}\right)^{\frac{1}{2}\mu} e^{-x} I_\mu(2\sqrt{xy}),$$

$$Q_{\mu+1}(x,y) = Q_\mu(x,y) + \left(\frac{y}{x}\right)^{\frac{1}{2}\mu} e^{-x} I_\mu(2\sqrt{xy}),$$

where $I_\mu(z)$ is the modified Bessel function.

Stability aspects are very important here.

From these recursions homogeneous four-term recursions can be derived for $P_\mu(x,y)$ and $Q_\mu(x,y)$.

Using special functions

The non-central chi-squared distributions

Integral representations are:

$$P_\mu(x,y) = e^{-x}\int_0^y \left(\frac{t}{x}\right)^{\frac{1}{2}(\mu-1)} e^{-t} I_{\mu-1}(2\sqrt{xt})\,dt,$$

$$Q_\mu(x,y) = e^{-x}\int_y^\infty \left(\frac{t}{x}\right)^{\frac{1}{2}(\mu-1)} e^{-t} I_{\mu-1}(2\sqrt{xt})\,dt.$$

Using special functions

The non-central chi-squared distributions

By using an integral representation of the Bessel function:

$$P_\mu(x,y) = \frac{e^{-x-y}}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{x/s+ys}}{(1-s)s^\mu}\,ds, \qquad c>1,$$

$$Q_\mu(x,y) = \frac{e^{-x-y}}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{x/s+ys}}{(1-s)s^\mu}\,ds, \qquad 0<c<1,$$

which in fact are inverse Laplace transforms.

They are useful for deriving uniform asymptotic expansions.

Using special functions

The non-central chi-squared distributions

In problems in radar communications very large values of μ, x, y are used, say, about 10,000.

Asymptotic analysis shows a transition when y passes the value $x + \mu$. There is a fast transition from 0 to 1.

The main approximant is in that case the complementary error function.

See T(1993) and T(1996).

Using special functions

A series of Bessel functions

Consider the series in terms of modified Bessel functions

$$\Phi(x,y) = -y - e^{\omega r \sin\theta} \sum_{n=-\infty}^{\infty} \frac{I_n'(\omega)}{I_n(\omega)}\, I_n(\omega r)\, \cos n(\theta + \pi/2).$$

The function $\Phi(x,y)$ is the solution of an elliptic boundary value problem inside a circle.

Using special functions

A series of Bessel functions

The equation reads

$$\varepsilon\left(\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}\right)-\frac{\partial\Phi}{\partial y}=1, \quad x^2+y^2<1,$$

with boundary condition

$$\Phi(\cos\theta,\sin\theta)=0$$

on the boundary of the circle $r=1$. We use polar coordinates

$$x=r\cos\theta, \quad y=r\sin\theta.$$

Using special functions

A series of Bessel functions

This is a so-called singular perturbation problem, ε is a small parameter.

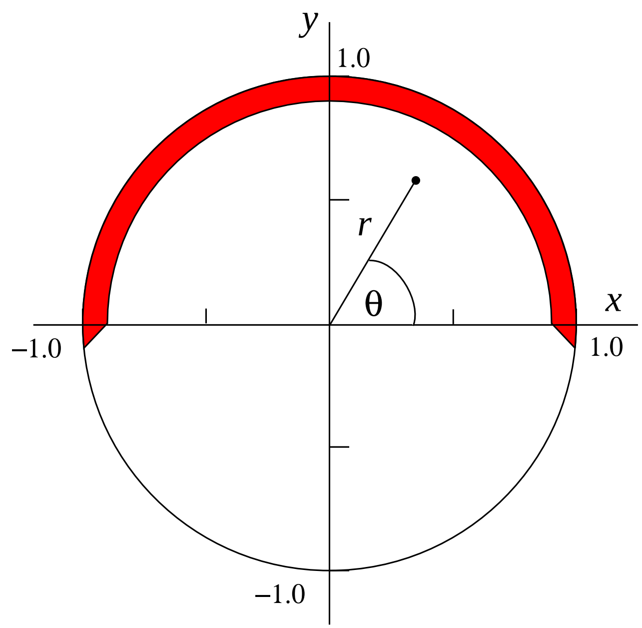
The solution has a boundary layer at the upper part of the circle.

We recall the solution, we write $\omega = \frac{1}{2\varepsilon}$,

$$\Phi(x, y) = -y - e^{\omega r \sin\theta} \sum_{n=-\infty}^{\infty} \frac{I_n'(\omega)}{I_n(\omega)} I_n(\omega r) \cos n(\theta + \pi/2).$$

Using special functions

A series of Bessel functions



Boundary layer inside the circle along the upper boundary $r = 1, y > 0$ and near the points $(\pm 1, 0)$.

Using special functions

A series of Bessel functions

It is difficult to compute Φ when $r \sim 1$ with $y > 0$, in particular in the neighborhoods of the points $(x, y) = (\pm 1, 0)$.

It is not difficult to compute the modified Bessel functions. But when ω is large, they become exponentially large, and the convergence of the Fourier series starts with high $n-$values.

In particular in the boundary layer large quantities are canceling before convergence starts.

Using special functions

A series of Bessel functions

A perturbation analysis starts with the expansion

$$\Phi(x,y) \sim \sum_{n=0}^{\infty} \varepsilon^n w_n(x,y)$$

in which the terms satisfy $\dfrac{\partial w_0(x,y)}{\partial y} = -1$, and

$$\frac{\partial w_n(x,y)}{\partial y} = \Delta w_{n-1}(x,y), \quad n = 1, 2, \ldots,$$

and all w_n should vanish at the lower part of the unit circle.

Using special functions

A series of Bessel functions

Integrating the first few relations for the w_j gives

$$w_0(x,y) = -y - R, \quad w_1(x,y) = \frac{y+R}{R^3},$$

$$w_2(x,y) = \frac{y+R}{2R^7}\left(3y + 12yx^2 + R\right),$$

where $R = \sqrt{1-x^2}$.

Observe that these w_n become singular at the points $(\pm 1, 0)$ and that they do not satisfy the boundary condition $w_n = 0$ on the upper part of the unit circle.

Using special functions

A series of Bessel functions

Simple model problems in singular perturbations with known exact solutions are of interest because

- Numerical codes for more general problems can be tested on these problems.
- They may give new challenges in (uniform) asymptotic analysis of integrals or series.
- They may provide asymptotic approximations that are difficult to obtain from perturbation analysis.

The series expansions of $\Phi(x, y)$ is a challenge for numerical computations.

Can we rely on Maple and Mathematica ?

Consider

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

- Maple 9.5, Digits = 10, for $\lambda = 10$, gives

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

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- With Digits = 40, the answer is

$$F(10) = -.1837516480532069664418890663053408790017+$$

$$+0.5305342892550606876095028928250448740020i.$$

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$$+0.5305342892550606876095028928250448740020i.$$

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

Can we rely on Maple and Mathematica ?

Take another integral, which is almost the same:

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

- Maple 9.5, Digits=10, for $\lambda = 10$, gives $G(10) = -0.1257674520 \times 10^{-15}$.

Can we rely on Maple and Mathematica ?

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- With Digits = 40, the answer is $G(10) = .16 \times 10^{-43}$.

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- Maple 9.5, Digits=10, for $\lambda = 10$, gives $G(10) = -0.1257674520 \times 10^{-15}$.
- With Digits = 40, the answer is $G(10) = .16 \times 10^{-43}$.
- The correct answer is $G(\lambda) = \sqrt{\pi} e^{-\lambda^2}$ and for $\lambda = 10$ we have $G(10) = 0.6593662989 \times 10^{-43}$.

Can we rely on Maple and Mathematica ?

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

Otherwise a completely incorrect answer can be accepted.

Mathematica is more reliable here, and says:

"NIntegrate failed to converge to prescribed accuracy after 7 recursive bisections in t near $t = 2.938461538461538 7$".

Can we rely on Maple and Mathematica ?

By the way, Maple 7 could do the following integral

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

and the funny answer was, after some simplification,

$$H(\lambda) = \sqrt{\pi}e^{-\lambda^2}[1 + \operatorname{signum}(t)\operatorname{erf} i\lambda],$$

where $\operatorname{erf} z$ is the error function.
In Maple 9.5 the answer is

$$H(\lambda) = \sqrt{\pi}e^{-\lambda^2}(1 + i\operatorname{erf}\lambda).$$

Can we rely on Maple and Mathematica ?

Consider

$$F(u) = \int_0^\infty e^{uit} \frac{dt}{t-1-i}, \quad u > 0.$$

Numerical quadrature gives $F(2) = -0.934349 - 0.70922i$.
Mathematica 4.1 gives for $u = 2$ in terms of the Meijer G-function:

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

Mathematica evaluates: $F(2) = -0.547745 - 0.532287i$.

Can we rely on Maple and Mathematica ?

Ask Mathematica to evaluate $F(u)$:

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

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

So, we have 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.

Can we rely on Maple and Mathematica ?

Maple 9.5:

$$F(u) = e^{iu-u}\mathrm{Ei}(1, iu-u) = e^{iu-u}\Gamma(0, iu-u),$$

same as Mathematica. This is a wrong answer.

Next, Maple 9.5, with $u = 2$,

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

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

Finally, ...

Thank You