Numerical Aspects of Special Functions

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- The complete revision of Abramowitz & Stegun (1964)

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The complete revision of A & S (1964)

- For the first time after the 1964 version a complete revision of Abramowitz and Stegun
- The new DLMF (Digital Library of Mathematical Functions) will appear in a hardcover edition and as a free electronic publication on the World Wide Web.
- New chapters on mathematical methods (such as computer algebra, asymptotic analysis) and new functions classes (such as $q-$hypergeometric functions, functions of matrix argument) will be included.
- This project started at NIST in 1999. It is expected now that the new book, the web version, and the CD version become available in 2006.

The complete revision of A & S (1964)

What to have at my desert island?

The complete revision of A & S (1964)

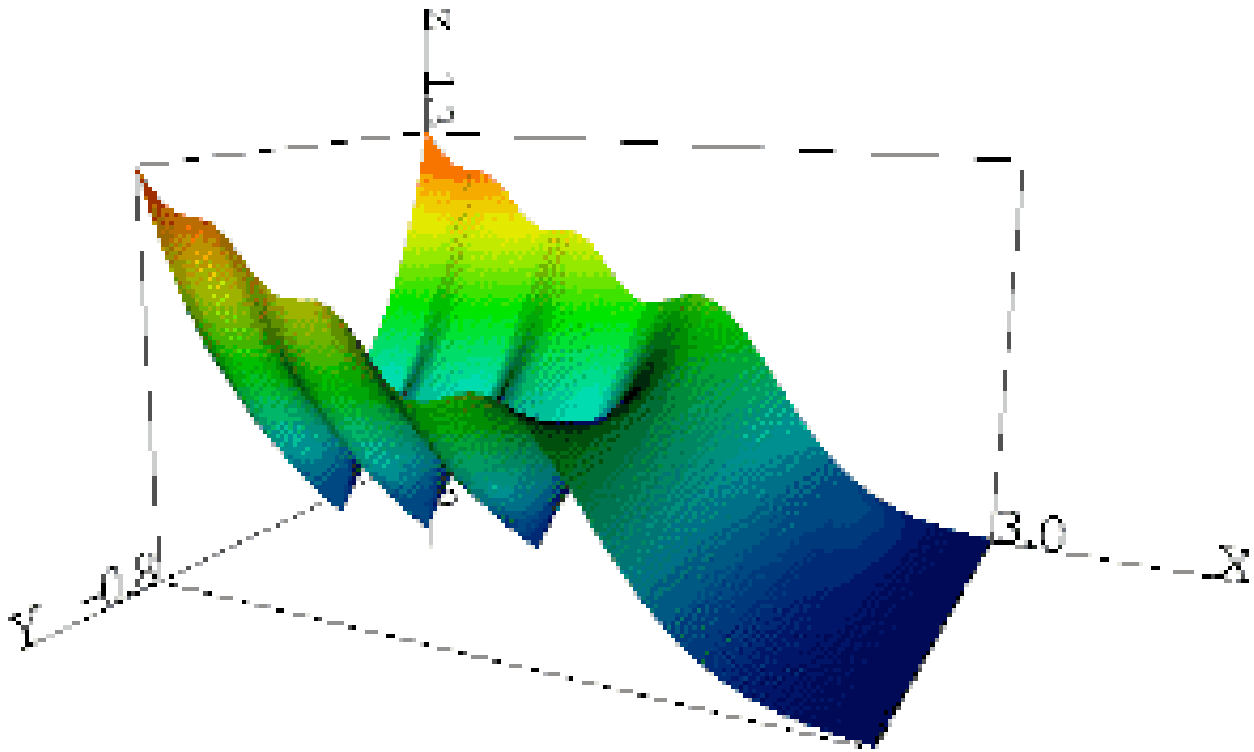

Figure 2: The Airy function $|\mathrm{Ai}(z)|$ in the complex plane

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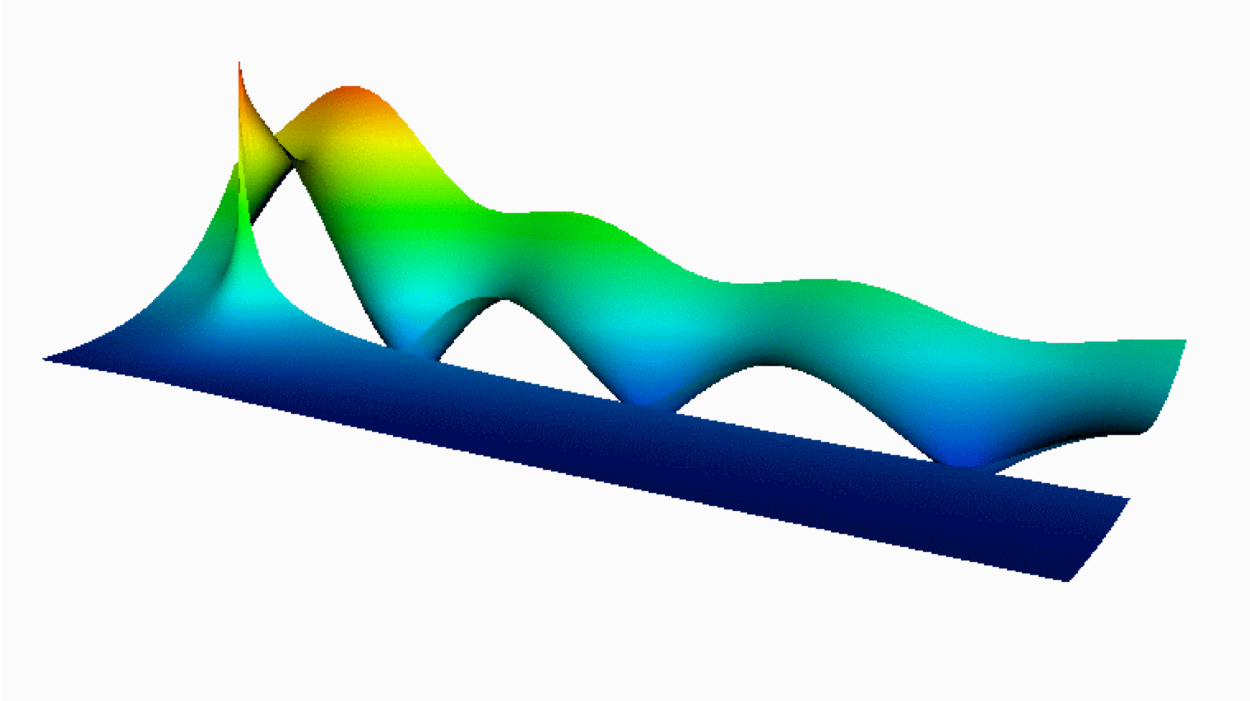

Figure 3: The Hankel function $|H_0^{(1)}(z)|$ in the complex plane

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 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 f_n and 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 f_0 and f_1 (forward recursion) is usually very unstable.

The solution g_n is called a dominant solution.

Recursion relations

For example, the functions

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

satisfy the recursion relation

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

Computing $f_n(1)$ 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 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.

The set of 26 recursions for ${}_2F_1-$ functions

The Gauss hypergeometric function is defined by

$$ {}_2F_1\left({a,\ b \atop c} ; z\right) = \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n\, n!}\, z^n, \qquad (a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}. $$

In this form it is defined for $|z| < 1$, and $c \neq 0, -1, -2, \ldots$.

Several recursion relations with respect to the parameters a, b, c exist. In fact, we have 26 relations for the functions

$$ y_n = {}_2F_1\left({a+\varepsilon_1 n,\ b+\varepsilon_2 n \atop c+\varepsilon_3 n} ; z\right), $$

where $\varepsilon_j = -1, 0, 1$ (not all $\varepsilon_j = 0$).

The set of 26 recursions for ${}_2F_1-$ functions

For example, the Gauss hypergeometric function

$$y_n = {}_2F_1\left(\begin{matrix} a+n, \ b \\ c \end{matrix}; z\right)$$

satisfies the recursion relation

$$(a+n)(z-1)y_{n+1}+(2a+2n-c-az-nz+bz)y_n+(c-a-n)y_{n-1} = 0.$$

There are important questions (from a numerical point of view).

The set of 26 recursions for ${}_2F_1-$ functions

Questions:

- Is this relation stable for computing this Gauss function? That is, can we compute $y_n, n \geq 2$, from y_0, y_1 in a stable way, or is y_n a minimal solution ?
- Can we find a second solution of this relation, and, if yes, is this solution a minimal or dominant solution ?
- Have these solutions the same properties (minimal, dominant) for all complex values of z ?

The set of 26 recursions for ${}_2F_1-$ functions

We consider recursion with respect to n of the hypergeometric function

$$ {}_2F_1\left(\begin{matrix} a+\varepsilon_1 n,\ b+\varepsilon_2 n \\ c+\varepsilon_3 n \end{matrix};\ z\right) $$

where

$$ \varepsilon_j = -1, 0, \text{or } 1. $$

There are $3^3 - 1 = 26$ possible recursions.

The set of 26 recursions for ${}_2F_1-$ functions

Because of the symmetry relation

$$ {}_2F_1\left(\begin{matrix} a,\ b \\ c \end{matrix};z\right) = {}_2F_1\left(\begin{matrix} b,\ a \\ c \end{matrix};z\right) $$

and the functional relation

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

only $\mathbf{5}$ basic forms need to be studied.

The remaining $\mathbf{21}$ recursions follow from these $\mathbf{5}$ recursions.

The set of 26 recursions for ${}_2F_1-$ functions

The basic forms are

$$ {}_2F_1\left(\begin{matrix} a+n,\ b+n \\ c \end{matrix};\ z\right), \quad {}_2F_1\left(\begin{matrix} a+n,\ b+n \\ c-n \end{matrix};\ z\right), $$

$$ {}_2F_1\left(\begin{matrix} a+n,\ b \\ c \end{matrix};\ z\right), \quad {}_2F_1\left(\begin{matrix} a+n,\ b \\ c-n \end{matrix};\ z\right), $$

$$ {}_2F_1\left(\begin{matrix} a,\ b \\ c+n \end{matrix};\ z\right). $$

The set of 26 recursions for ${}_2F_1-$ functions

It is also important to consider the following three cases

$$ {}_2F_1\left(\begin{matrix} a, \ b \\ c-n \end{matrix} ; z\right), $$

$$ {}_2F_1\left(\begin{matrix} a-n, \ b \\ c+n \end{matrix} ; z\right), $$

$$ {}_2F_1\left(\begin{matrix} a-n, \ b-n \\ c+n \end{matrix} ; z\right), $$

which follow from the five basic forms by changing the n–direction.

The set of 26 recursions for ${}_2F_1-$ functions

Remember the theory of the Gauss differential equation. The six functions

$$w_1 = {}_2F_1\left({a,\ b \atop c};z\right), \qquad w_2 = z^{1-c}{}_2F_1\left({1+a-c,\ 1+b-c \atop 2-c};z\right),$$

$$w_3 = {}_2F_1\left({a,\ b \atop a+b+1-c};1-z\right), \qquad w_4 = (1-z)^{c-a-b}{}_2F_1\left({c-a,\ c-b \atop c+1-a-b};1-z\right),$$

$$w_5 = (z^{-1}e^{i\pi})^a{}_2F_1\left({a,\ a+1-c \atop a+1-b};\frac{1}{z}\right), \quad w_6 = (z^{-1}e^{i\pi})^b{}_2F_1\left({b,\ b+1-c \atop b+1-a};\frac{1}{z}\right)$$

satisfy the same differential equation.

The set of 26 recursions for ${}_2F_1-$ functions

Each w_j can be written as a linear combination of two other w–functions. For example

$$w_1 = \frac{\Gamma(a+1-c)\Gamma(b+1-c)}{\Gamma(1-c)\Gamma(a+b+1-c)} w_3 - \frac{\Gamma(a+1-c)\Gamma(b+1-c)\Gamma(c-1)}{\Gamma(1-c)\Gamma(a)\Gamma(b)} w_2.$$

The set of 26 recursions for ${}_2F_1-$ functions

Observations:

- Each term in the right-hand side satisfies the same differential equation as $\mathbf{w_1}$.
- Each term in the right-hand side satisfies the same difference equation as $\mathbf{w_1}$.
- Hence, by considering several linear combinations, we can find several solutions of the same difference equation (recursion relation).

The set of 26 recursions for ${}_2F_1-$ functions

Given the recursion relation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0$$

we compute

$$\alpha = \lim_{n\to\infty} a_n, \quad \beta = \lim_{n\to\infty} b_n,$$

and consider the characteristic polynomial

$$t^2 + \alpha t + \beta = 0$$

with zeros t_1 and t_2.

The set of 26 recursions for ${}_2F_1-$ functions

Then, if $|t_1| \neq |t_2|$, the difference equation has two linear independent solutions f_n and g_n with the properties

$$\frac{f_{n+1}}{f_n} \sim t_1, \qquad \frac{g_{n+1}}{g_n} \sim t_2.$$

If $|t_1| > |t_2|$, we call f_n a dominant solution, and g_n the minimal solution.

The set of 26 recursions for ${}_2F_1-$ functions

For all hyper recursions, t_1 and t_2 do not depend on a, b, c; they may depend on z.

For all hyper recursions, t_1 and t_2 are non-zero and finite (except for some simple z–values).

By verifying when $|t_1| = |t_2|$, we find domains in the complex z–plane where we have to identify minimal and dominant solutions of the five basic recursion relations.

The set of 26 recursions for ${}_2F_1$ — functions

The recursion for ${}_2F_1\left(\begin{matrix} a+n,\ b+n \\ c \end{matrix}; z\right)$.

There is a pair $\{f_n, g_n\}$ with

$$\lim_{n\to\infty} \frac{f_{n+1}}{f_n} = t_1 = \frac{1}{(1-\sqrt{z})^2},$$

$$\lim_{n\to\infty} \frac{g_{n+1}}{g_n} = t_2 = \frac{1}{(1+\sqrt{z})^2},$$

The equation $|t_1| = |t_2|$ holds when $z \le 0$. The function related with w_3 is minimal; the other five functions related with the other w_j are dominant.

The set of 26 recursions for ${}_2F_1-$ functions

In this case we have

$$y_1 = {}_2F_1\left(\begin{matrix} a+n,\ b+n \\ c \end{matrix}; z\right),$$

$$y_3 = \frac{\Gamma(a+n+1-c)\Gamma(b+n+1-c)}{\Gamma(a+b+2n+1-c)}\,{}_2F_1\left(\begin{matrix} a+n,\ b+n \\ a+b+2n+1-c \end{matrix}; 1-z\right).$$

When z is not on the negative real axis:
y_1 is dominant, y_3 is minimal.

The set of 26 recursions for ${}_2F_1-$ functions

The Jacobi polynomial is a special case:

$$P_n^{(\alpha,\beta)}(x) = \binom{n+\alpha}{n} \left(\frac{1+x}{2}\right)^{\alpha+\beta+n+1} {}_2F_1\left({\alpha+1+n,\ \alpha+\beta+n+1 \atop \alpha+1}; \frac{x-1}{x+1}\right)$$

Forward recursion is not unstable for $P_n^{(\alpha,\beta)}(x)$ when $x \in [-1,1]$.

The set of 26 recursions for ${}_2F_1$— functions

The recursion for ${}_2F_1\left({a+n,\, b+n \atop c-n};\, z\right)$.

There is a pair $\{f_n, g_n\}$ with

$$\lim_{n\to\infty} \frac{f_{n+1}}{f_n} = t_1 = \frac{32(1+w)}{(3+w)^3},$$

$$\lim_{n\to\infty} \frac{g_{n+1}}{g_n} = t_2 = \frac{32(1-w)}{(3-w)^3},$$

where $w = \sqrt{1+8z}$. The equation

$$|t_1| = |t_2|$$

holds on the curve shown in Figure 4.

The set of 26 recursions for ${}_2F_1-$ functions

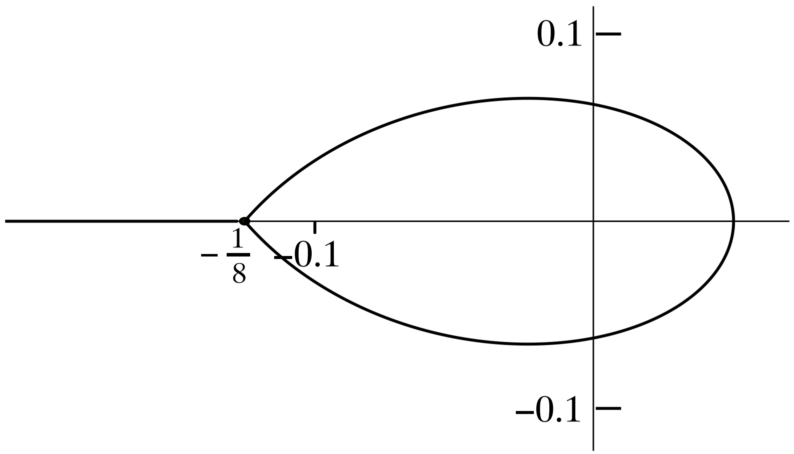

Figure 4: The curve $|t_1| = |t_2|$ for the case $(+\,+\,-)$.

The function y_2 related with w_2 is minimal in the domain inside the curve; the function related with w_3 is minimal in the domain outside the curve; the other functions related with the other w_j are dominant.

The set of 26 recursions for ${}_2F_1-$ functions

The corresponding y_1 (always dominant), y_2, y_3 for this case:

$$y_1 = {}_2F_1\left(\begin{matrix} a+n,\ b+n \\ c-n \end{matrix}; z\right),$$

$$y_2 = (-z)^n \frac{\Gamma(b+1-c+2n)\Gamma(a+1-c+2n)}{\Gamma(a+n)\Gamma(b+n)\Gamma(1-c+n)\Gamma(2-c+n)} \times$$

$${}_2F_1\left(\begin{matrix} 1+a-c+2n,\ 1+b-c+2n \\ 2-c+n \end{matrix}; z\right),$$

$$y_3 = \frac{\Gamma(b+1-c+2n)\Gamma(a+1-c+2n)}{\Gamma(1-c+n)\Gamma(a+b+1-c+3n)}\, {}_2F_1\left(\begin{matrix} a+n,\ b+n \\ a+b+1-c+3n \end{matrix}; 1-z\right).$$

The set of 26 recursions for ${}_2F_1-$ functions

The recursion for ${}_2F_1\left(\begin{matrix} a+n,\ b \\ c \end{matrix}; z\right)$.

There is a pair $\{f_n, g_n\}$ with

$$\lim_{n\to\infty} \frac{f_{n+1}}{f_n} = t_1 = 1,$$

$$\lim_{n\to\infty} \frac{g_{n+1}}{g_n} = t_2 = \frac{1}{1-z}$$

The equation

$$|t_1| = |t_2|$$

holds on the curve shown in Figure 5, a circle with centre 1 and radius 1.

The set of 26 recursions for ${}_2F_1-$ functions

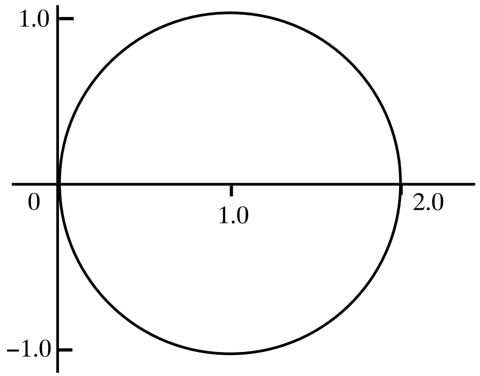

Figure 5: The curve $|t_1| = |t_2|$ for the case $(+\,0\,0)$.

The function related with w_3 is minimal inside the circle; the function related with w_5 is minimal outside the circle; the other functions related with the other w_j are dominant.

The set of 26 recursions for ${}_2F_1-$ functions

The y_1 (always dominant), y_3, y_5 for this case:

$$y_1 = {}_2F_1\left(\begin{matrix} a+n,\ b \\ c \end{matrix}; z\right),$$

$$y_3 = \frac{\Gamma(a+n+1-c)}{\Gamma(a+b+n+1-c)}\,{}_2F_1\left(\begin{matrix} a+n,\ b \\ a+b+n+1-c \end{matrix}; 1-z\right),$$

$$y_5 = (-z)^{-n}\frac{\Gamma(n+1-c+a)}{\Gamma(1+a+n-b)}\,{}_2F_1\left(\begin{matrix} a+n,\ a+n+1-c \\ a+n+1-b \end{matrix}; \frac{1}{z}\right).$$

The set of 26 recursions for ${}_2F_1-$ functions

The recursion for ${}_2F_1\left({a+n,\ b \atop c-n};z\right)$.

There is a pair $\{f_n, g_n\}$ with

$$\lim_{n\to\infty}\frac{f_{n+1}}{f_n} = t_1 = 1,$$

$$\lim_{n\to\infty}\frac{g_{n+1}}{g_n} = t_2 = -\frac{4z}{(1-z)^2}.$$

The equation

$$|t_1| = |t_2|$$

holds on the curve shown in Figure 6.

The set of 26 recursions for ${}_2F_1-$ functions

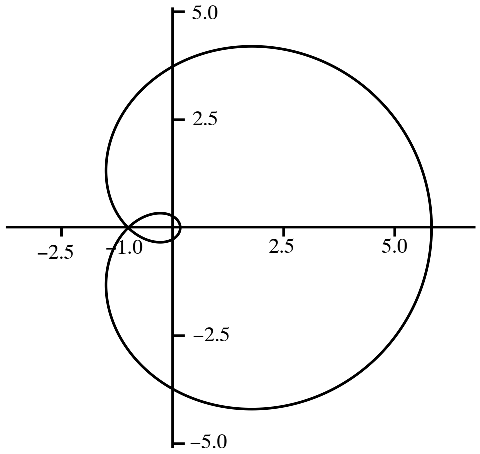

Figure 6: The curve $|t_1| = |t_2|$ for the case $(+\,0\,-)$.

The function related with w_2 is minimal in the domain inside the inner curve; the function related with w_3 is minimal in the domain between the two curves; the function related with w_5 is minimal in the domain outside the outer curve; the other functions related with the other w_j are dominant.

The set of 26 recursions for ${}_2F_1-$ functions

The y_1 (always dominant), y_2, y_3, y_5 for this case:

$$y_1 = {}_2F_1\left(\begin{matrix} a+n,\ b \\ c-n \end{matrix}; z\right),$$

$$y_2 = (-z)^n \frac{\Gamma(b+1-c+n)\Gamma(a+1-c+2n)}{\Gamma(a+n)\Gamma(1-c+n)\Gamma(n+2-c))} {}_2F_1\left(\begin{matrix} 1+a-c+2n,\ 1+b-c+n \\ 2-c+n \end{matrix}; z\right),$$

$$y_3 = \frac{\Gamma(b+1-c+n)\Gamma(a+1-c+2n)}{\Gamma(1-c+n)\Gamma(a+b+1-c+2n)} {}_2F_1\left(\begin{matrix} a+n,\ b \\ a+b+1-c+2n \end{matrix}; 1-z\right),$$

$$y_5 = (-z)^{-n} \frac{\Gamma(1+a-c+2n)}{\Gamma(1-c+n)\Gamma(1+a-b+n)} {}_2F_1\left(\begin{matrix} a+n,\ a+1-c+2n \\ a+1-b+n \end{matrix}; \frac{1}{z}\right).$$

The set of 26 recursions for ${}_2F_1-$ functions

The recursion for ${}_2F_1\left({a,\ b \atop c+n}; z\right)$.

There is a pair $\{f_n, g_n\}$ with

$$\lim_{n\to\infty}\frac{f_{n+1}}{f_n}=t_1=1,\qquad \lim_{n\to\infty}\frac{g_{n+1}}{g_n}=t_2=\frac{z-1}{z}.$$

The equation $|t_1|=|t_2|$ holds when $\Re z=\frac{1}{2}$. The function related with w_1 is minimal when $\Re z<\frac{1}{2}$; the function related with w_4 is minimal when $\Re z>\frac{1}{2}$; the other functions related with the other w_j are dominant.

The set of 26 recursions for ${}_2F_1-$ functions

The $\boldsymbol{y_1}$, $\boldsymbol{y_4}$ for this case:

$$y_1 = {}_2F_1\left(\begin{matrix} a, \ b \\ c+n \end{matrix}; z\right),$$

$$y_4 = (z-1)^n \frac{\Gamma(n+c)}{\Gamma(c+1-a-b+n)} \times$$

$$ {}_2F_1\left(\begin{matrix} c+n-a, \ c+n-b \\ c+n+1-a-b \end{matrix}; 1-z\right).$$

The set of 26 recursions for ${}_2F_1-$ functions

The $(0\;0\;-),(-\;0\;+),(-\;\;-\;\;+)$ recursions:

These recursions need extra attention, although they are "negative n" cases of some of the basic forms.

The domains for these recursions are the same as those for the $(0\;0\;+),(+\;0\;-),(+\;\;+\;\;-)$ cases, respectively, which we have done earlier.

However, for each case (and each domain) the minimal and dominant solutions have to be identified again.

The set of 26 recursions for ${}_2F_1-$ functions

Conclusions (so far):

- We have identified minimal and dominant solutions for all 26 recursion relations for the hypergeometric functions.
- We have described the domains in the complex z–plane where these minimal and dominant solutions have been identified.
- Proofs of these properties (not mentioned in this lecture) are available, and are based on behaviour of solutions near the singular points $\mathbf{0, 1, \infty}$ of the Gauss differential equation.

The set of 26 recursions for ${}_2F_1$— functions

Literature:

- Papers on recursions (theory): Wong & Li (1992a,b).
- Papers on recursions (numerics): Gautschi (1967), Olver (1967).
- Book on recursions: Wimp (1984).
- Books on asymptotics: Olver, Wong, Luke.
- Recent papers on asymptotics of Gauss functions: Jones, Olde Daalhuis, Temme.
- Paper on numerics of Gauss functions: Forrey (1997).
- Project on recursion of Kummer functions: Deaño & Segura (2005).
- Papers on recursion of Legendre functions:
  Gil & Segura (1997, 1998, ...).
- Two papers on recursion of Gauss hypergeometric functions:
  Gil, Segura, Temme (JCAM, ??).

Power series to compute Gauss functions ?

Consider the following questions.

1. Can we compute the Gauss hypergeometric function by using power series and the many transformations that are available for this function?
2. Can we compute this function for all possible values of a, b and c?

Power series to compute Gauss functions ?

How to compute the Gauss function ?

- Power series
- Integrals
- Differential equation
- Recursion relations
- Chebychev expansions
- Continued fractions

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Power series to compute Gauss functions ?

The standard power series is

$$ {}_2F_1\left(\begin{matrix} a, & b \\ & c \end{matrix}; z\right) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n\, n!} z^n, \qquad |z| < 1. $$

Together with relations such as

$$ {}_2F_1\left(\begin{matrix} a, & b \\ & c \end{matrix}; z\right) = (1-z)^{-a} {}_2F_1\left(\begin{matrix} a, & c-b \\ & c \end{matrix}; \frac{z}{z-1}\right). $$

For this function with need, when we use its power series,

$$ \left|\frac{z}{z-1}\right| < 1. $$

Power series to compute Gauss functions ?

In several other ways we can write the Gauss function in terms of other Gauss functions.
The new arguments are

$$\frac{1}{z}, \quad 1-z, \quad \frac{1}{1-z}, \quad \frac{z}{z-1}, \quad \frac{z-1}{z}.$$

Power series to compute Gauss functions ?

For numerical computations we need convergence conditions like

$$|z| < \rho,\ \left|\frac{1}{z}\right| < \rho,\ |1-z| < \rho,\ \left|\frac{1}{1-z}\right| < \rho,\ \left|\frac{z}{z-1}\right| < \rho,\ \left|\frac{z-1}{z}\right| < \rho,$$

with

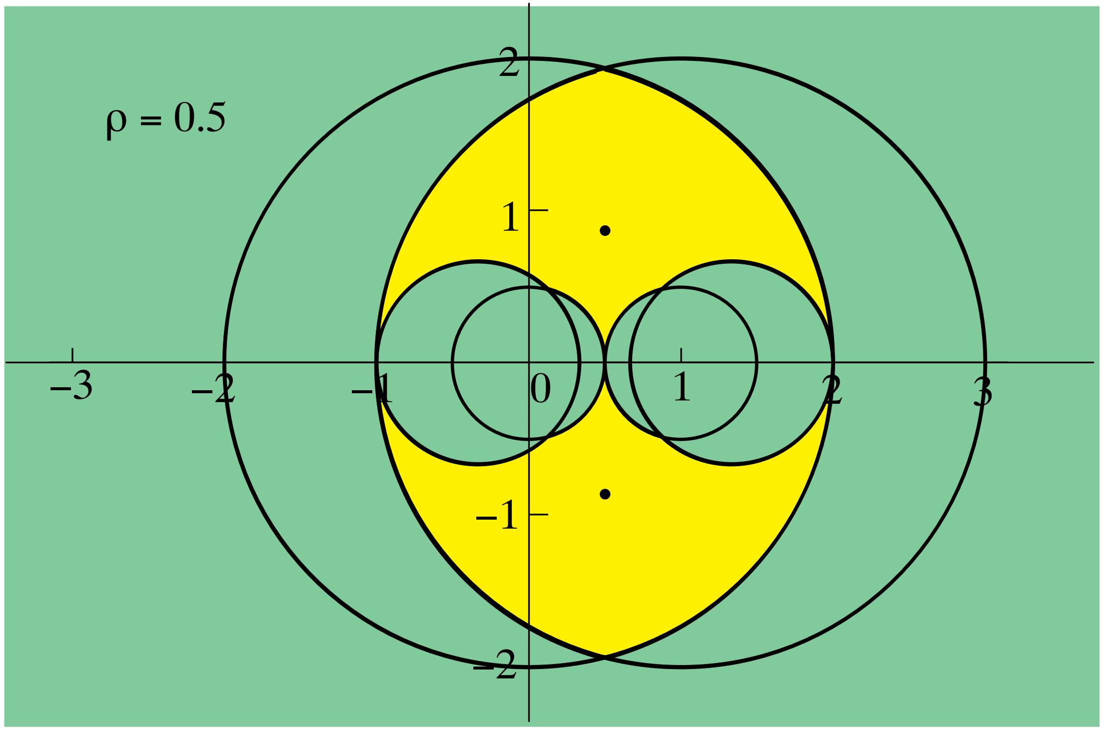
$$0 < \rho < 1.$$

Power series to compute Gauss functions ?

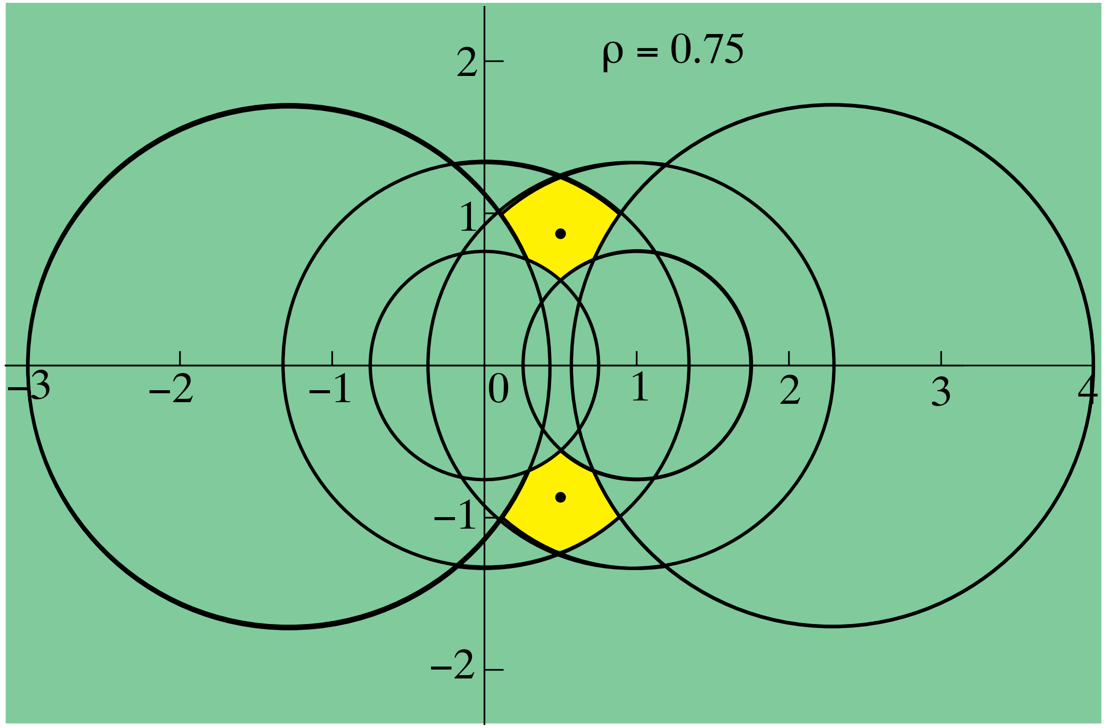
Can we cover the whole $z-$plane with some number ρ?
In the green domain one of the conditions

$$|z| < \rho,\ \left|\frac{1}{z}\right| < \rho,\ |1-z| < \rho,\ \left|\frac{1}{1-z}\right| < \rho,\ \left|\frac{z}{z-1}\right| < \rho,\ \left|\frac{z-1}{z}\right| < \rho$$

is satisfied. This is the case $\rho = 0.5$.



Power series to compute Gauss functions ?



This is the case $\rho = 0.75$.

In the yellow domains, 'around' the points $e^{\pm\frac{1}{3}\pi i}$, the standard power series cannot be used with this value of ρ.

Power series to compute Gauss functions ?

Other pitfalls:

- For large values of a or b instabilities arise, and the power series converge slowly.
- For certain combinations of a, b and c removable singularities occur.

Power series to compute Gauss functions ?

Example $c = a + b$:

$$
{}_2F_1\left({a,\ b \atop c};z\right) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\,{}_2F_1\left({a,\ b \atop a+b-c+1};1-z\right) +
$$

$$
\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\,{}_2F_1\left({c-a,\ c-b \atop c-a-b+1};1-z\right).
$$

This relation is well defined for $c = a + b$ because singularities are cancelled.
If $c \sim a + b$ numerical computations are not stable.

Power series to compute Gauss functions ?

Summarizing so far:

- power series are very efficient in certain domains of the complex plane
- not all $z-$values can be covered
- instabilities occur for certain values of the parameters.

Numerical quadrature for special functions

The standard integral representations of special functions are not always suitable for numerical computations.

When parameters are large, integrals with oscillatory integrands can be very unstable representations.

By using complex contours for these integrals, or for transformed versions, stable representations can be obtained.

Numerical quadrature to compute special functions

The next task is selecting a suitable quadrature rule for computations.

Because the integrands are analytic functions, high-precision quadrature rules can be selected.

Numerical quadrature to compute special functions

Example: 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	$-.53\ 10^{-404}$

Much better than the standard estimates of R_n.
Explanation: periodicity and smoothness.

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

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$$+0.5305342892550606876095028928250448740020i.$$

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- 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 $G(10) = -0.1257674520 \times 10^{-15}$.

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- 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 $t = 2.9384615384615387$".

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,

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

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

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

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.

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 of this talk.

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

The project is not finished yet and the publication date is not known yet.

To be published by SIAM.