On the numerical evaluation of functions and related topics

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Seminario MATESCO

Contents:

Elementary functions and operations:

1. +,-,*,/
2. Polynomials
3. Trigonometric
4. Exponential and logarithm

Elementary functions (trigonometric functions, exponential, log):

algorithms based on polynomial approximation and/or table lookup; Shift-and-Add algorithms.

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Enough?
Of course, not.
There is "a bunch" of useful functions which do not fall inside this narrow category. To mention few:

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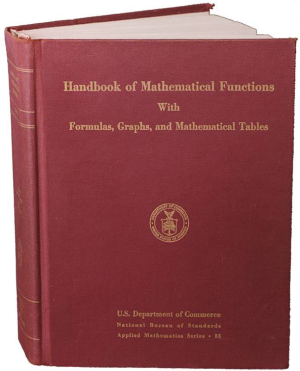
3. The Airy functions: solutions of $y''(z) - zy(z) = 0$
4. And many more, some of them depending on several parameters (hypergeometric functions among them)

Are these elementary functions? Why not?

A & S: a best seller



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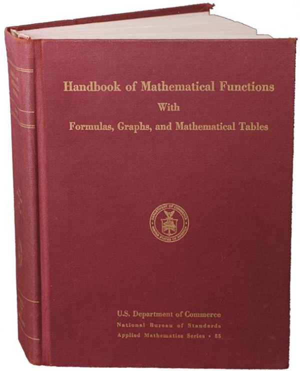
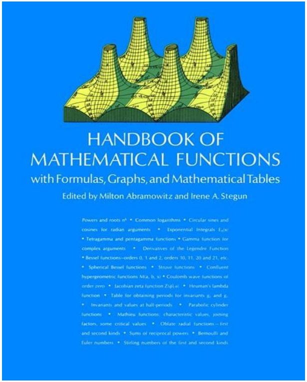
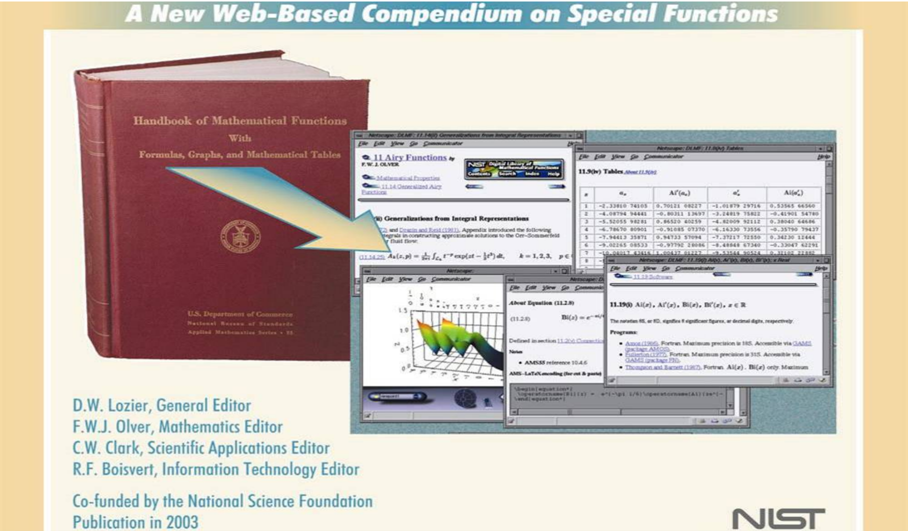




A & S needs a revision



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On June 11, 2008, Dan Lozier (NIST) wrote:

- A 5-chapter preview of the DLMF has been installed on the public web site http://dlmf.nist.gov .
- It contains all the intended functionality of the eventual full public release, now scheduled for late this year or early next.
- Visitors to the web site are invited to give feedback about the current status.

Airy functions

Airy functions are the solution of the ODE:

The Airy equation

$$y''(z) - zy(z) = 0$$

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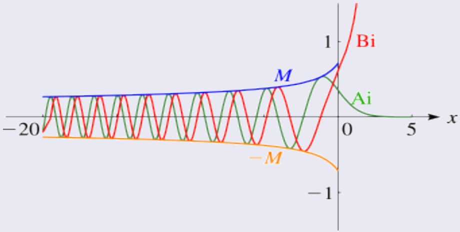

The goal: computing a numerically satisfactory pair of solutions of the Airy equation for real $z > 0$. A numerically satisfactory pair should comprise the recessive solution.

We try power series and get two independent solutions:

$$y_1(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{1}{3}\right)_k \frac{z^{3k}}{(3k)!}, \quad y_2(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{2}{3}\right)_k \frac{z^{3k+1}}{(3k+1)!}$$

where $3^k(\alpha + 1/3)_k = (3\alpha + 1)(3\alpha + 4) \cdots (3\alpha + 3k - 2)$

The series converge in $\mathbb{C}$. Good. Have we finished?

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No, we haven't: $\lim_{z\to+\infty} y_1(z) = +\infty$, $\lim_{z\to+\infty} y_2(z) = +\infty$, and we need the solution $\mathrm{Ai}(z)$ such that $\lim_{z\to+\infty} \mathrm{Ai}(z) = 0$.

Of course, we have some α, β such that

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But this is bad conditioned! **Computing a small quantity from two large quantities leads to disaster.**

Now, we transform the equation $y'' - zy = 0$ by considering the functions $Y(z) = z^{1/4}y(z)$, which, in the variable $\zeta = 2/3z^{3/2}$, satisfy the ODE

$$\ddot{Y}(\zeta) + \left[-1 + \frac{5}{36\zeta^2}\right] Y(\zeta) = 0$$

This suggest that $Y(\zeta) \sim e^{\pm\zeta}$ as $\zeta \to +\infty$ (Liouville-Green approximation).

This, in turn, tells us that $\mathrm{Ai}(z) \sim Kz^{-1/4}e^{-2/3z^{3/2}}$.

For a better approximation, write $Y(\zeta) = e^{-\zeta}g(\zeta)$. Now $g(\zeta)$ satisfies

$$\frac{d^2g}{d\zeta^2} - 2\frac{dg}{d\zeta} + \frac{\lambda}{\zeta^2}g = 0, \quad \lambda = \frac{5}{36},$$

and using a formal series in powers of ζ^{-1}, that is, $g(\zeta) = \sum_{k=0}^{\infty} a_m\zeta^{-m}$, we get, equating term by term,

$$a_{m+1} = -\frac{\lambda + m(m+1)}{2(m+1)}a_m, \quad m = 0, 1, 2, \ldots .$$

Therefore, we find the expansion

$$\mathrm{Ai}(z) \sim z^{-1/4} e^{-\zeta} \sum_{m=0}^{\infty} a_m \zeta^{-m}, \quad \zeta = \frac{2}{3} z^{3/2}, a_0 = (2\sqrt{\pi})^{-1}$$

The series is divergent for any ζ, but has asymptotic nature.
It can be shown that this an asymptotic expansion for $\mathrm{Ai}(z)$ for large $|z|$ except when z is real and $\Re(z) < 0$.
A second independent solution is

$$\mathrm{Bi}(z) \sim 2z^{-1/4} e^{\zeta} \sum_{m=0}^{\infty} (-1)^m a_m \zeta^{-m},$$

Asymptotic expansions

When we say that an expansion of the form

$$f(z) \sim \sum_{n=0}^{\infty} a_n z^{-n}, \quad z \to \infty$$

is an *asymptotic expansion*, we assume that

$$z^N \left(f(z) - \sum_{n=0}^{N-1} a_n z^{-n} \right), \quad N = 0, 1, 2, \ldots,$$

where the sum is empty when $N = 0$, is a bounded function for large values of z, with limit a_N as $z \to \infty$, for any N. This can also be written as

$$f(z) = \sum_{n=0}^{N-1} a_n z^{-n} + \mathcal{O}\left(z^{-N}\right), \quad z \to \infty.$$

The validity is usual restricted to a sector in the $z-$plane

A first algorithm

We have two possible approximations: for z small and large. Can we match them?

1. Small positive z ▸ Convergent series
2. Large positive z ▸ Divergent series

Indeed, we get 10^{-8} relative precision using convergent series for $z < 5.5$ and divergent series for $z > 5.5$.
For more precision, we need something new.
Before this, let us stress some important points.

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2. Also, it is convenient to determine the dominant factors ($\exp(\pm 2/3z^{3/2}$ for Airy functions).
3. When it is possible to factor out these dominant factors and we can do it for a satisfactory pair of solutions, we can say that we have given a totally satisfactory solution, particularly when the scaled-out functions can be numerically computed for any z.

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We can not expect to compute a function numerically with a single method unless the functions is quite elementary.

For improving the computation of Airy functions, additional approximations shoud be considered for intermediate z. Some possibilities:

1. Chebyshev expansions (for real z only)
2. Numerical quadrature (for $z \in \mathbb{C}$) [Gil, Segura, Temme 2002]
3. Numerical integration of the ODE (for $z \in \mathbb{C}$) [Fabijonas, Olver, Lozier 2004]

Let us describe the last two methods (ODE solving very briefly).

In Fabijonas, Lozier and Olver, the computation of Airy functions by solving the initial value problem is considered (they use Taylor's method).

A crucial point is the conditioning of the integration.

Because $\lim_{z\to+\infty} \mathrm{Ai}(z)/\mathrm{Bi}(z) = 0$, one should never compute numerically $\mathrm{Ai}(z)$ integrating from $z = 0$.

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For $\mathrm{Ai}(z)$ the problem must be put this way:

Compute $\mathrm{Ai}(x)$ in $[0, b]$ starting from the know values $\mathrm{Ai}(b)$ and $\mathrm{Ai}'(b)$.

For b large enough $\mathrm{Ai}(b)$ and $\mathrm{Ai}'(b)$ can be approximated with the asymptotic expansions.

Again, it is necessary to have information on the behavior of the solutions before trying any numerical method.

Many (special functions) can be written using integral representations, also Airy functions. Two representations are:

$$\mathrm{Ai}(z) = \frac{1}{\pi}\int_0^{+\infty} \cos(t^3/3 + zt)dt$$

$$\mathrm{Ai}(z) = \frac{1}{\sqrt{\pi}(48)^{1/6}\Gamma(5/6)} e^{-\zeta}\zeta^{-1/6}\int_0^{+\infty}\left(2+\frac{t}{\zeta}\right)^{-1/6} t^{-1/6}e^{-t}dt$$

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Which one is the best for numerical purposes?

The second one does not have an oscillating integrand and shows explictly the main factor

Steepest descent as a tool for oscillatory integrands

Consider the numerical computation of

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Straightforward computation by using any quadrature rule is very unstable when λ is large.

Shift the path of integration upwards in the complex $t-$plane to make it run through the point $t = i\lambda$, or write

$$-t^2 + 2i\lambda t = -(t - i\lambda)^2 - \lambda^2.$$

This gives

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

or, by writing $t = i\lambda + s$,

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

In this simple example we deform the original contour of integration to let it run through the saddle point.

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In this simple example we deform the original contour of integration to let it run through the saddle point.
This method can be used for many special functions defined by real or contour integrals.

Numerical quadrature: Airy functions

A complex contour integral for the Airy function:

We consider

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

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

Numerical quadrature: Airy functions

Let

$$\phi(w) = \tfrac{1}{3} w^3 - zw.$$

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

$$\Im[\phi(w)] = \Im[\phi(w_0)].$$

We write

$$z = x + iy = re^{i\theta}, \quad w = u + iv, \quad w_0 = u_0 + iv_0.$$

Then

$$u_0 = \sqrt{r} \cos \tfrac{1}{2}\theta, \quad v_0 = \sqrt{r} \sin \tfrac{1}{2}\theta, \quad x = u_0^2 - v_0^2, \quad y = 2u_0 v_0.$$

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

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

Numerical quadrature: Airy functions

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

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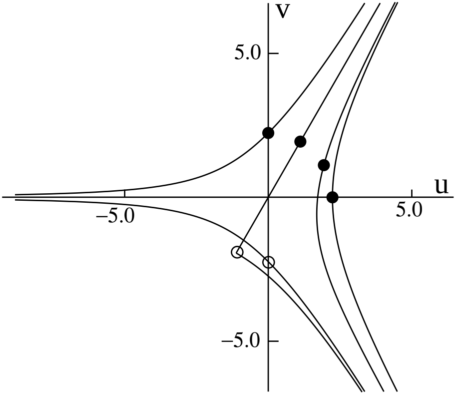
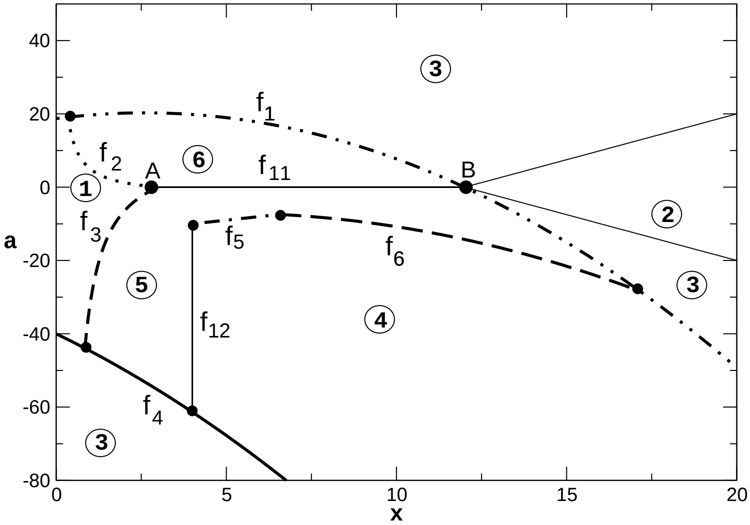


A pair of additional examples

We have solved in a numerical satisfacory way some other problems, like:

1. Solution of the Bessel equation $x^2y'' + xy + (x^2 + a^2)y = 0$ (2004)
2. Solution of the parabolic cylinder equation $y'' + (a - x^2/4)y = 0$ (2006)

This problems are harder because they involve the variable x and the parameter a, and a completelly satisfactory solution must be so in the (a, x) plane. A good number of methods are usually needed.
Just to have an idea of the difficulty, here are the regions where different methods are used for the parabolic cylinder equation:



40
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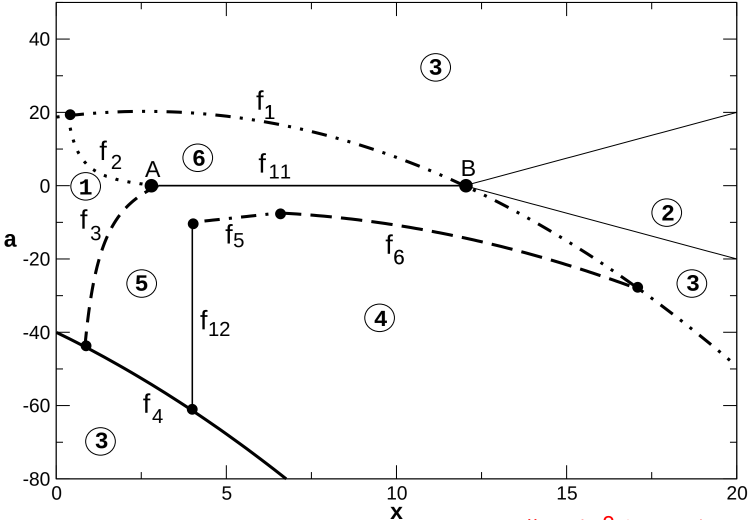

Now we are working on the harder case $y'' + (x^2/4 - a)y = 0$

Recurrence relations

In the previous figure, in one of the regions the following relation is used:

$$U(a-1,x) = xU(a,x) + (a+1/2)U(a+1,x)$$

This is a three-term recurrence relation (a difference equation of 2nd order)

Recurrence relations are simple methods of computation when starting values are known.

But they should be handled with care!

Recurrence relations: a simple example

Consider

$$y_{n+1} - 2\cosh(x) y_n + y_{n-1} = 0,\ x > 0$$

which has a solution $y_n = exp(-nx)$.
We start from $y_0 = 1$, $y_1 = e^{-1}$ and compute numerically up to $n = 40$.

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We should get $y_{40}/y_{39} = e^{-1}$, but we get

$$y_{40}/y_{39} = 2.71828182845905$$

Why? Because $y_n = exp(nx)$ is also a solution, which dominates over $exp(-nx)$ (which is said to be minimal).
Again, a conditioning problem arises and we need to have information on the solutions.

Recurrence relations: not so simple results

In Gil, Segura and Temme, Math. Comput. (2007), the conditioning of Gauss hypergeometric recursions was analyzed. A result

Around $z = 0$ the functions

$$y_n = {}_2F_1(a + \epsilon_1 n, b + \epsilon_2 n; c + \epsilon_3 n; z)$$

are minimal solutions as $n \to +\infty$ of the corresponding TTRR if and only if $\epsilon_3 > 0$. The minimality holds in the open connected region including $z = 0$ where the **characteristic roots** have different moduli.

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In the same paper, all the cases with $|\epsilon_i| \leq 1$ are analyzed.

More recently (Segura, Temme, Num. Math. 2008) the problem for confluent hypergeometric functions has been solved for any $\epsilon_i \in \mathbb{Z}$.

No time for:

1. High order methods for solving nonlinear equations
2. Qualitative properties of the zeros of special functions
3. Convergence and pseudoconvergence of continued fractions associated to three-term recurrence relations.

Maybe some other day.

Numerical software

- A wide survey of the available software: Lozier & Olver (1994); last update: December 2000. [Needs a new update.]
  http://math.nist.gov/mcsd/Reports/2001/nesf/paper.pdf
- Interactive systems based on computer algebra:
  Matlab, Maple, Mathematica.
- Mathematical libraries:
  CALGO, SLATEC, CERN, IMSL, NAG.
- Books with software:
  Baker, Moshier, Numerical Recipes, Thompson, Wong & Guo, Zhang & Jin.

  And now, also our book (see http://functions.unican.es)