

Recent developments in the computation of special functions

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Elementary functions:

- 1 Polynomials, algebraic functions
- 2 Trigonometric and inverses
- 3 Exponential and logarithm

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5 The error function: $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$

6 The Airy functions: solutions of $y''(z) - zy(z) = 0$, particularly

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Less elementary functions are, for instance, hypergeometric functions (Kummer, Gauss). Call them special if you wish.



Our principles for computing (special) functions:

- 1 The main objective is to develop Fortran codes which produce reliable double precision values. Generally, we don't use Maple or Mathematica in the final product.
- 2 A given special function is usually a special case of a more general function. Our approach is bottom-up: starting from the simplest cases. For example: Airy functions.
- 3 We accept that it is necessary to combine several methods in order to compute a function accurately and efficiently for a wide range of its variables.
- 4 We accept that a theoretical error analysis is usually impossible for functions with several real or complex variables. We accept more empirical approaches.
- 5 The accuracy analysis is usually done by using functional relations, such as a Wronskian relations or by comparing with an alternative method of computation.
- 6 The selection of methods in different parameter domains is based on speed and accuracy, where the latter may prevail.
- 7 Possible scaling factors may be considered when available

An example: Airy functions

Airy functions are the solutions of the ODE:

The Airy equation

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

Relatively recent methods for computing this function in the complex plane are:

- 1 Fabijonas, Lozier, Olver (ACM TOMS 2004)
- 2 Gil, Segura, Temme (ACM TOMS 2002)

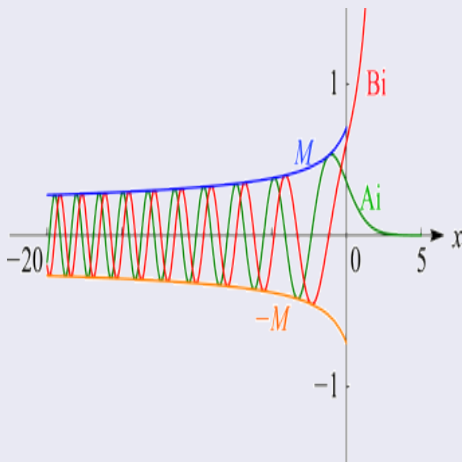
The goal: computing a **numerically satisfactory pair** of solutions of the Airy equation for unrestricted values of the variable (possibly factoring out an elementary function). A numerically satisfactory pair should comprise the recessive solution ($Ai(z)$ is recessive as $|z| \rightarrow \infty$, $\arg(z) < \pi/3$).

I am describing briefly the case of $Ai(z)$, starting with positive real z .

An example: Airy functions

Airy functions are the solutions of the ODE:

The Airy equation



For small x : we try power series and get two independent solutions:

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

But $\lim_{z \rightarrow +\infty} y_1(z) = +\infty$, $\lim_{z \rightarrow +\infty} y_2(z) = +\infty$, while $\lim_{x \rightarrow +\infty} \text{Ai}(x) = 0$. The computation of $\text{Ai}(x)$ for large x is numerically unstable using convergent series.

For large x asymptotics can be used.

$$\text{Ai}(z) \sim z^{-1/4} e^{-\zeta} \sum_{m=0}^{\infty} a_m \zeta^{-m}, \quad \zeta = \frac{2}{3} z^{3/2}, \quad a_{m+1} = -\frac{5/36 + m(m+1)}{2(m+1)} a_m, \quad a_0 = (2\sqrt{\pi})^{-1}$$

A first algorithm: use convergent series for $x < 5.5$ and divergent series for $x > 5.5$ (10^{-8} relative precision).

For more precision, we need something else. **We can not expect to compute a function numerically with a single method unless it is quite elementary.**

Something else: Chebyshev expansions, integration of the ODE, **numerical quadrature**,...

Numerical quadrature

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

$$\text{Ai}(z) = \frac{1}{2\pi i} \int_{\infty e^{-i\pi/3}}^{+\infty e^{i\pi/3}} \exp(t^3/3 - zt) dt$$

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

Which one is the best for numerical purposes?

Numerical quadrature

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

$$\text{Ai}(z) = \frac{1}{2\pi i} \int_{-\infty e^{-i\pi/3}}^{+\infty e^{i\pi/3}} \exp(t^3/3 - zt) dt$$

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Which one is the best for numerical purposes?

The second one does not have an oscillating integrand and shows explicitly the dominant factor.

But the first integral can be transformed by complex integration methods (saddle point analysis).



Numerical quadrature: a trivial example of contour deformation

$$I = \int_{-\infty}^{+\infty} \cos(w^2/2 + xw) dw = \Re(F),$$

$$F = \int_{-\infty}^{+\infty} e^{\phi(w)} dw, \quad \phi(t) = i(w^2/2 + xw)$$

$$\phi'(w_0) = 0 \rightarrow w_0 = -x$$

The path $w = v - x + iv$, $v \in (-\infty, +\infty)$ is of steepest descent (SD) and one can deform the original path to the SD path, where $dw = (1 + i)dv$, $\Re(\phi(w)) = -v^2$ and:

$$F = \int_{-\infty}^{+\infty} e^{\phi(w)} dw = e^{\phi(w_0)}(1 + i) \int_{-\infty}^{+\infty} e^{-v^2} dv$$

The remaining integral is suited for the trapezoidal rule (not needed).
With this $F = e^{-ix^2/2}(1 + i)\sqrt{\pi}$ and $I = \sqrt{2\pi} \cos(x^2/2 - \pi/4)$.

For Airy:

$$\text{Ai}(z) = \frac{1}{2\pi i} \int_C e^{\frac{1}{3}w^3 - zw} dw, \quad \text{ph } z \in [0, \frac{2}{3}\pi]$$

C : contour starting at $\infty e^{-i\pi/3}$ and terminating at $\infty e^{+i\pi/3}$ (in the valleys of the integrand).

Let

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

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

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

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

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

The resulting integral is suited for the trapezoidal rule.

Our recipe for complex Airy functions:

- 1 Maclaurin series.
- 2 Asymptotic expansions
- 3 Gauss-Laguerre quadrature (but also the trapezoidal rule)

Recurrence relations

Many special functions satisfy difference equations, and in particular,

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

Examples: $U(a, x)$ and $V(a, x)$ ($a \equiv n$) or $P_{-1/2+i\tau}^m(x)$ ($m \equiv n$)

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Example: Consider the recurrence $y_{n+1} - y_n - y_{n-1} = 0$, (Fibonacci) with general solution $y_n = \alpha\phi^n + \beta(-\phi^{-1})^n$, $\phi = (1 + \sqrt{5})/2$.

Consider the numerical computation of the $(-\phi)^{-n}$ starting from $y_0 = 1$, $y_1 = -2/(1 + \sqrt{5})$. We compute up to $n = 50$.

We should get $y_{50}/y_{49} = -2/(1 + \sqrt{5})$, but we get $y_{50}/y_{49} = 1.618150\dots$

The solution $y_n = \phi^n$ dominates over $(-\phi^{-1})^n$ (minimal). Any small numerical error introduces the dominant solution. This is a conditioning problem; **we need information on the conditioning of the solutions.**

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Similar precautions have to be considered when integrating initial value problems for ODEs.



Recurrences: main results to be considered

- 1 Perron-Kreuser theorem, which essentially says that for a linear difference equation of order k , $y_{n+k+1} + a_n^{(n+k)}y_{n+k} + \dots + a_n^{(0)}y_n = 0$ there exist different solutions such the ratios y_{n+1}/y_n behave as $n \rightarrow +\infty$ as the solutions of the characteristic equation $\lambda^{n+k+1} + a_n^{(n+k)}\lambda^{n+k} + \dots + a_n^{(0)} = 0$ (in the non-degenerate case).
- 2 The asymptotic behaviour of the solution we want to compute, to be compared with the Perron-Kreuser predictions. Is the solution recessive (minimal), dominant or none of them?
- 3 Pincherle's theorem for three term recurrence relations:
 $y_{n+1} + b_n y_n + a_n y_{n-1} = 0$ has minimal solution $\{f_n\}$ if and only if:

$$\frac{f_n}{f_{n-1}} = \frac{-a_n}{b_n + \frac{-a_{n+1}}{b_{n+1} + \dots}}$$

Additional examples of computation

We (AG, NT and myself) have solved some other problems, like:

- 1 Various types of Legendre functions of real parameters (1997,1998,2000)
- 2 Inhomogeneous Airy functions (2000).
- 3 Solution of the Bessel equation $x^2 y'' + xy + (x^2 + a^2)y = 0$ (2004). Numerically satisfactory pair $\{K_{ia}(x), L_{ia}(x)\}$.
- 4 Solution of the parabolic cylinder equation $y'' + (a \pm x^2/4)y = 0$ (2006 for $-$, 2011 and 2012 for $+$). Pairs of solutions $\{U(a, x), V(a, x)\}$ ($-$ case) and $\{W(a, x), W(a, -x)\}$
- 5 Conical functions, that is, Legendre functions $P_{-1/2+ir}^m(x)$ (2009, 2012).
- 6 Incomplete gamma functions $\gamma(a, x), \Gamma(a, x)$ (2012)

The last four problems are harder because they involve two or more variables. A good number of methods are usually needed to cover a large range.

Computation of χ^2 cumulative distributions

Recent activity involves the computation and inversion of χ^2 cumulative distributions.

The central distributions are given by the incomplete gamma function ratios

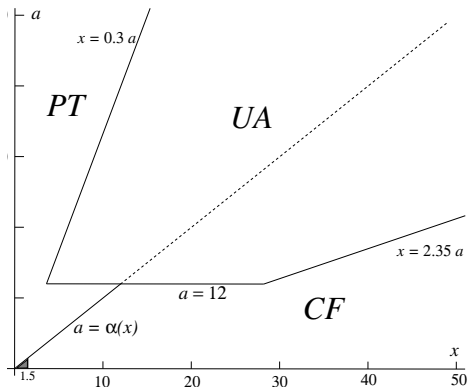
$$P(a, x) = \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t} dt, \quad Q(a, x) = \frac{1}{\Gamma(a)} \int_x^{+\infty} t^{a-1} e^{-t} dt$$

Because $P(a, x) + Q(a, x) = 1$ we only need to compute one function. We compute the smallest of the two.

For large values of a, x we have a transition at $a \sim x$, with

$$P(a, x) \lesssim \frac{1}{2} \quad \text{when} \quad a \gtrsim x,$$
$$Q(a, x) \lesssim \frac{1}{2} \quad \text{when} \quad a \lesssim x.$$

Accordingly, the methods of computation are divided in two zones, with several methods of computation in each one.



PT: Taylor series for P

QT: Taylor series for Q (small triangle)

UA: Uniform asymptotic expansions (Temme, 1979)

CF: continued fraction for the Q (Gautschi, 1977)

See A. Gil, JS, N.M. Temme, SIAM J. Sci. Comput. (2012)

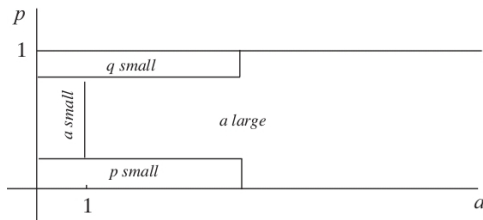
Inversion of the cumulative central χ^2 distribution

For probability distributions, the inversion is also needed in applications. For fixed a , we invert $P(a, x) = p$ or, equivalently, $Q(a, x) = q$.

Our approach:

- 1 Invert $P(a, x)$ ($Q(a, x)$) if $p < q$ ($p > q$)
- 2 Use the existent approximation methods (PT, Poincaré asymptotics for Q , UA) to find starting values.
- 3 Apply higher order Newton methods from the resulting starting values.

The different type of starting values are chosen according to the next figure.



An example of inversion:

For small p , we use PT to write

$$x = r \left(1 + \sum_{n=1}^{\infty} \frac{a(-1)^n x^n}{(a+n)n!} \right)^{-1/a}, \quad r = (p\Gamma(1+a))^{1/a},$$

We write $x = r + \sum_{n=2}^{\infty} c_n r^n$, and by expanding the first few coefficients are

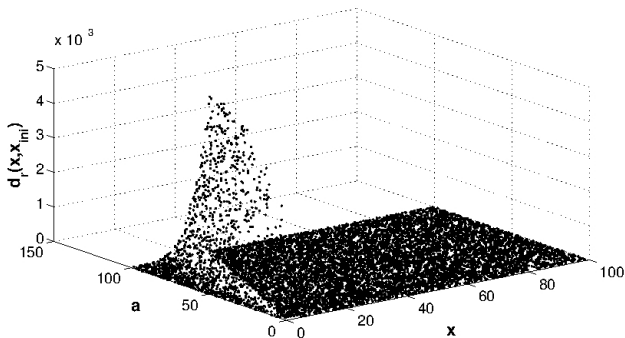
$$c_2 = \frac{1}{a+1},$$

$$c_3 = \frac{3a+5}{2(a+1)^2(a+2)},$$

$$c_4 = \frac{8a^2 + 33a + 31}{3(a+1)^3(a+2)(a+3)},$$

$$c_5 = \frac{125a^4 + 1179a^3 + 3971a^2 + 5661a + 2888}{24(1+a)^4(a+2)^2(a+3)(a+4)}.$$

The accuracy of the starting values (except for small a) is shown in this figure



With a fourth order Newton-like method, 2 or 3 iterations are enough for an accuracy better than 10^{-12} .

The generalized Marcum Q-function

The generalized Marcum Q-function is the **non-central cumulative χ^2 distribution**, up to an elementary change of variables. It is defined as

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

where $\mu > 0$ and $I_\mu(z)$ is the modified Bessel function. For $\mu = 1$ the function is known as the Marcum Q-function.

We also use a complementary function such that $P_\mu(x, y) + Q_\mu(x, y) = 1$:

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

Particular values are

$$Q_\mu(x, 0) = 1, \quad Q_\mu(x, +\infty) = 0,$$

$$Q_\mu(0, y) = Q_\mu(y), \quad Q_\mu(+\infty, y) = 1,$$

$$Q_{+\infty}(x, y) = 1.$$

As for incomplete gamma functions, we compute the smallest of the two functions. Asymptotic analysis gives that for large values of μ, x, y , we have a transition at $y \sim x + \mu$, with

$$P_\mu(x, y) \lesssim Q_\mu(x, y) \quad \text{when} \quad y \lesssim x + \mu,$$

$$Q_\mu(x, y) \lesssim P_\mu(x, y) \quad \text{when} \quad y \gtrsim x + \mu.$$

Ingredients in the computation:

- 1 Series in terms of incomplete gamma functions
- 2 Recurrence relations.
- 3 Asymptotic expansions for large μ in terms of the error function (both for P and Q).
- 4 Quadrature methods.

We give some details of the first two items.

Series in incomplete gamma functions

Plugging the Maclaurin series for the modified Bessel function into the integral representation, we readily obtain the series expansions

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

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

in terms of the incomplete gamma function ratios (which we can compute). Recurrences can be used to compute rapidly the series. We have

$$Q_{\mu+1}(y) = Q_\mu(y) + \frac{y^\mu e^{-y}}{\Gamma(\mu + 1)},$$

$$P_{\mu+1}(y) = P_\mu(y) - \frac{y^\mu e^{-y}}{\Gamma(\mu + 1)},$$

stable for $Q_\mu(y)$ in the forward direction, and for $P_\mu(y)$ in the backward direction. Equivalently, we have $\mu Q_{\mu+1}(y) - (\mu + y)Q_\mu(y) + yQ_{\mu-1}(y) = 0$.

Recurrence relations

Integration by parts gives the following recurrences

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

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

It is possible to eliminate the Bessel function and obtain a homogeneous third order recurrence relation.

$$xQ_{\mu+2}(x, y) = (x - \mu)Q_{\mu+1}(x, y) + (y + \mu)Q_{\mu}(x, y) - yQ_{\mu-1}(x, y),$$

and $P_{\mu}(x, y)$ satisfies the same relation, but its computation with this recurrence is badly conditioned (it is subdominant, but not minimal)

A better possibility is:

$$y_{\mu+1} - (1 + c_{\mu})y_{\mu} + c_{\mu}y_{\mu-1} = 0, \quad c_{\mu} = \sqrt{\frac{y}{x}} \frac{I_{\mu}(2\sqrt{xy})}{I_{\mu-1}(2\sqrt{xy})}.$$

P is minimal and Q is dominant. Pincherle's theorem gives:

$$\frac{P_{\mu}(x, y)}{P_{\mu-1}(x, y)} = \frac{c_{\mu}}{1 + c_{\mu}} - \frac{c_{\mu+1}}{1 + c_{\mu+1}} - \dots$$



The methods are combined as follows:

Let $f_1(x, \mu) = x + \mu - 0.25\sqrt{4x + 2\mu}$, $f_2(x, \mu) = x + \mu + 0.25\sqrt{4x + 2\mu}$.

- 1 If $\mu > 60$, compute the Marcum functions using either with asymptotic expansions for $f_1(x, \mu) < y < f_2(x, \mu)$ and use numerical quadrature in the other case.
- 2 If $\mu \leq 60$, compute the Marcum functions as follows:
 - If $\mu \leq 10$, $x < 15$, $y < 15$, compute the series expansion.
 - In other case: if $y < f_1(x, \mu)$ or $y > f_2(x, \mu)$ compute by numerical quadrature; if $f_1(x, \mu) < y < f_2(x, \mu)$ compute the Marcum functions using the recurrence relation.

The algorithm has been implemented in a Fortran 90 module **MarcumQ**, which includes the Fortran 90 routine **marcum** for the computation of $Q_\mu(x, y)$ and $P_\mu(x, y)$. We have tested that an accuracy $\sim 10^{-12}$ can be obtained in the parameter region $(x, y, \mu) \in [0, 200] \times [0, 200] \times [1, 200]$ (submitted to ACM Trans. Math. Softw.)

Inversion of the generalized Marcum Q -function

For a three variable function, we have to fix what we mean by inversion. It appears that in applications the inversion process is as follows (Helstrom, 1998):

We are given two numbers q_0, q_1 , both in $(0, 1)$, and we assume a fixed value of m .

Step 1: Find y from the equation $Q_\mu(0, y) = q_0$, and denote this value with y_0 . Because $Q_\mu(0, y) = Q_\mu(y)$ (the normalized incomplete gamma function) we already know how to do this step.

Step 2: Find x from the equation $Q_\mu(x, y_0) = q_1$, and denote this value with x_1 . The value y_0 is obtained in Step 1.

Ingredients of the inversion algorithm

- 1 Asymptotic inversion for large μ .
- 2 Analyze the converge of Newton or secant methods, not only for large μ .

For the second purpose: we need to analyze monotonicity and convexity. We have

$$\frac{\partial Q(x, y)}{\partial x} = Q_{\mu+1}(x, y) - Q_{\mu}(x, y) = \left(\frac{y}{x}\right)^{\mu/2} e^{-x-y} I_{\mu}(2\sqrt{xy}) > 0$$

Taking the second derivative and using the TTRR

$$\frac{\partial^2 Q(x, y)}{\partial x^2} = (c_{\mu}(x, y) - 1)(Q_{\mu+1}(x, y) - Q_{\mu}(x, y))$$

It is easy to prove that $c_{\mu}(x, y)$ is monotonically decreasing a a function of x , and using that (JS, J. Math. Anal. Appl., 2011)

$$f_{\mu+1}(z) < \frac{1}{z} \frac{I_{\mu}(z)}{I_{\mu-1}(z)} < f_{\mu+1/2}(z), \quad f_{\nu}(z) = (\nu + \sqrt{\nu^2 + z^2})^{-1}$$

we see that

$$\begin{aligned} \frac{\partial^2 Q}{\partial x^2} &< 0 \text{ if } x > x^+ = y - \mu - \frac{1}{2}, \\ \frac{\partial^2 Q}{\partial x^2} &> 0 \text{ if } x < x^- = y - \mu - 1 \end{aligned}$$

Consequence: for solving the second step (computing x in $Q(x, y) = q_1$), x^- and x^+ are safe starting values for the secant method when they are positive. Otherwise, taking two small positive values is safe.

Computation of the zeros of special functions

The problem: given a **function with several zeros** in an interval, compute all the zeros reliably and efficiently.

Reliability: no zero is missed and the method is convergent without accurate initial approximations.

Efficiency: the total count of iterations is small (and if the order of convergence is high so much the better).

We solve the problem for a wide set of functions which includes many important cases (like computing the zeros of orthogonal polynomials for Gauss quadrature, computing the zeros of Bessel functions and of their derivatives,...).

Most published algorithms rely on first approximations + Newton method.

Reliable?: maybe (therefore, certainly not). There is no proof of convergence.

Efficient?: yes, but can be improved without additional computational cost.

Additionally, one needs particular approximations for each different function and sometimes they are hard.

The initial approximations are difficult to handle for functions depending on several parameters (say Jacobi polynomials).

“Our” SFs:

Solutions of linear second order ODEs

$$w''(x) + B(x)w'(x) + C(x)w(x) = 0 \quad (1)$$

In particular, we will consider equations in normal form

$$y''(x) + A(x)y(x) = 0$$

We can transform (1) by setting

$$y(x) = \exp\left(\int \frac{1}{2}B(x)dx\right) w(x)$$

Then $y''(x) + A(x)y(x) = 0$, with $A(x) = C(x) - \frac{1}{2}B'(x) - \frac{1}{4}B(x)^2$



Construction of a fixed point method of order 4

Taking $h(x) = y(x)/y'(x)$, we have $h'(x) = 1 + A(x)h(x)^2$.

If $y(\alpha) = 0$ and $A(x)$ has slow variation:

$$\int_{\alpha}^x \frac{h'(\zeta)}{1 + A(\zeta)h(\zeta)^2} d\zeta \approx x - \alpha,$$

and assuming $A(x) > 0$

$$\alpha \approx x - \frac{1}{w(x)} \arctan(w(x)h(x)), \quad w(x) = \sqrt{A(x)}$$

A classroom exercise:

Prove that the fixed point method $x_{n+1} = g(x_n)$,

$$g(x) = x - \frac{1}{\sqrt{A(x)}} \arctan\left(\sqrt{A(x)} \frac{y(x)}{y'(x)}\right)$$

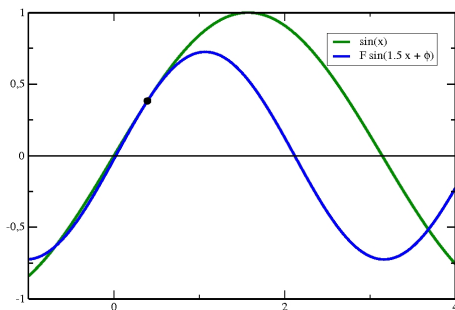
with $y''(x) + A(x)y(x) = 0$, $A(x)$ differentiable, has order of convergence four.

But the goal is to compute all the zeros in a given interval. How to be sure?



Theorem (Sturm comparison)

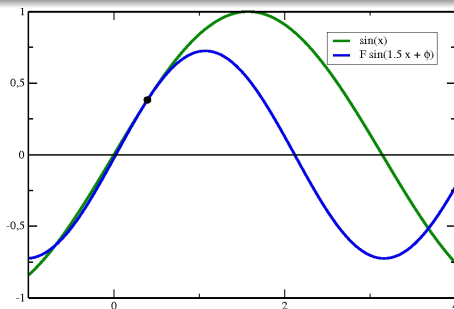
Let $y(x)$ and $w(x)$ be solutions of $y''(x) + A_y(x)y(x) = 0$ and $w''(x) + A_w(x)w(x) = 0$ respectively, with $A_y(x) > A_w(x) > 0$. If $y(x_0)w'(x_0) - y'(x_0)w(x_0) = 0$ and x_y and x_w are the zeros of $y(x)$ and $w(x)$ closest to x_0 and larger (or smaller) than x_0 , then $x_y < x_w$ (or $x_y > x_w$).



Equations: $y''(x) + y(x) = 0$, $y''(x) + 2.25y(x) = 0$

Algorithm (Zeros of $y''(x) + A(x)y(x) = 0$, $A(x)$ monotonic)

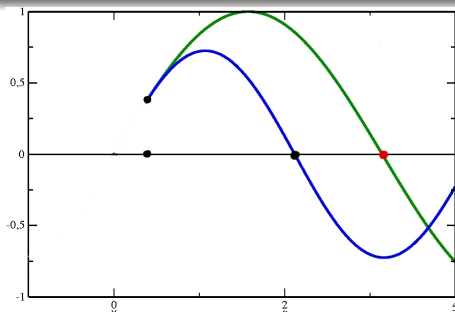
Given x_n , the next iterate x_{n+1} is computed as follows: find a solution of the equation $w''(x) + A(x_n)w(x) = 0$ such that $y(x_n)w'(x_n) - y'(x_n)w(x_n) = 0$. If $A'(x) < 0$ ($A'(x) > 0$) take as x_{n+1} the zero of $w(x)$ closer to x_n and larger (smaller) than x_n .



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Algorithm (Zeros of $y''(x) + A(x)y(x) = 0$, $A(x)$ monotonic)

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Equations: $y''(x) + A(x)y(x) = 0$, $w''(x) + A(x_n)w(x) = 0$, ($A'(x) < 0$)

The method is equivalent to iterating $x_{n+1} = T(x_n)$ with the following fixed point iteration.

Let $j = \text{sign}(A'(x))$, we define

$$T(x) = x - \frac{1}{\sqrt{A(x)}} \arctan_j(\sqrt{A(x)}h(x))$$

with

$$\arctan_j(\zeta) = \begin{cases} \arctan(\zeta) & \text{if } jz > 0, \\ \arctan(\zeta) + j\pi & \text{if } jz \leq 0, \\ j\pi/2 & \text{if } z = \pm\infty \end{cases}$$

This method converges to α for any x_0 in $[\alpha', \alpha)$ if $A'(x) < 0$, with α' the largest zero smaller than α (analogously for $A'(x) > 0$).

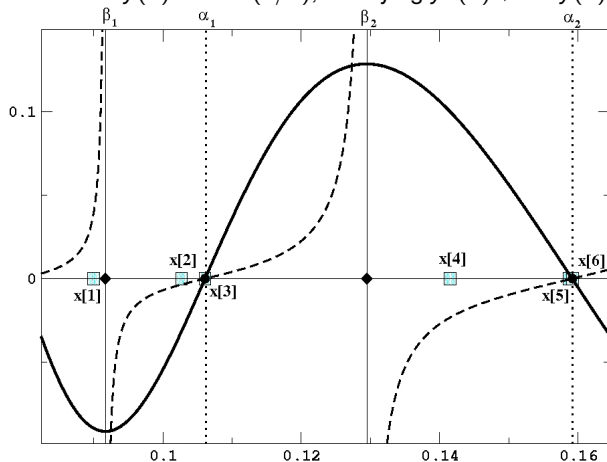
The method has fourth order convergence:

$$\epsilon_{n+1} = \frac{A'(\alpha)}{12} \epsilon_n^4 + \mathcal{O}(\epsilon_n^5), \quad \epsilon_k = x_k - \alpha$$



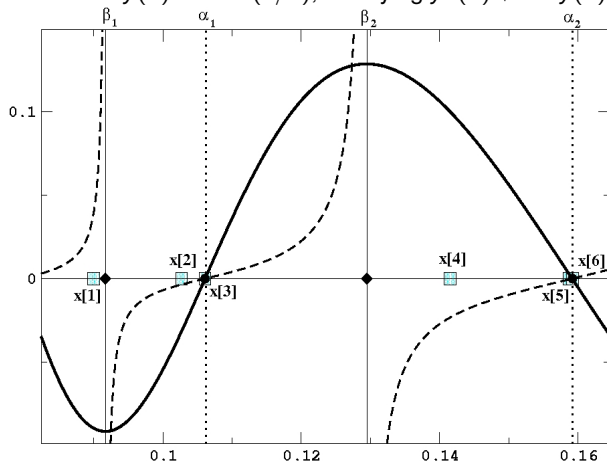
Computing the zeros in an interval where $A(x)$ is monotonic.

Example: zeros of $y(x) = x \sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



Computing the zeros in an interval where $A(x)$ is monotonic.

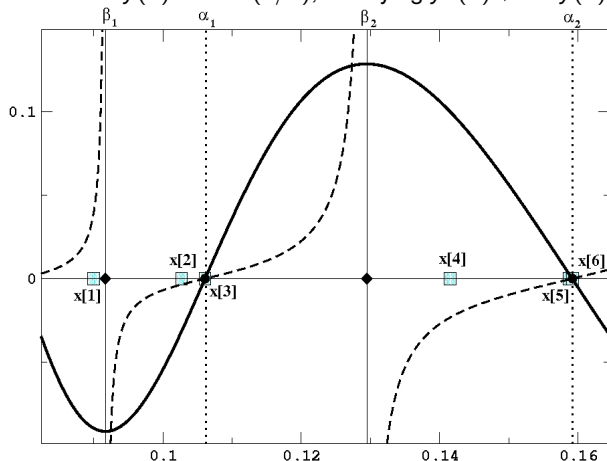
Example: zeros of $y(x) = x \sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



1 $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)

Computing the zeros in an interval where $A(x)$ is monotonic.

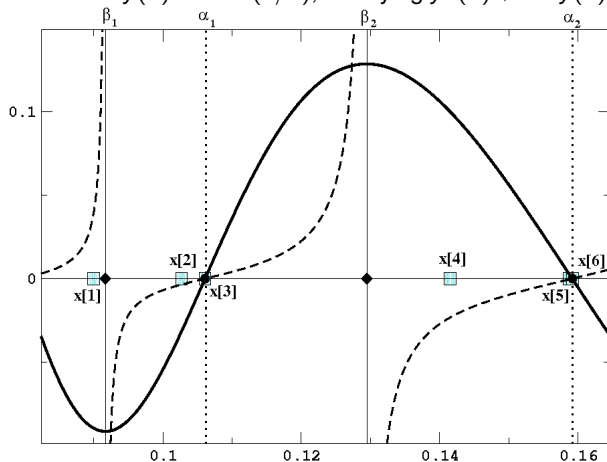
Example: zeros of $y(x) = x \sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



- 1 $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)
- 2 $x[4] = x[3] + \pi / \sqrt{A(x[3])}$ (smaller than the next zero by Sturm comparison)

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- 1 $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)
- 2 $x[4] = x[3] + \pi / \sqrt{A(x[3])}$ (smaller than the next zero by Sturm comparison)
- 3 $T(x[4]) = x[5]$, $T(x[5]) = x[6]$ (with four digits acc.)

The algorithm

The basic algorithm is as simple as this:

Algorithm

Computing zeros for $A'(x) < 0$

- 1 Iterate $T(x)$ starting from x_0 until an accuracy target is reached. Let α be the computed zero.
- 2 Take $x_0 = T(\alpha) = \alpha + \pi/\sqrt{A(\alpha)}$ and go to 1.

Repeat until the interval where the zeros are sought is swept. For $A'(x) > 0$ the same ideas can be applied but the zeros are computed in decreasing order.

See JS, SIAM J. Numer. Anal. (2010).

Requirement: the monotonicity properties of $A(x)$ should be known in advance in order to compute zeros in sub-intervals where $A(x)$ is monotonic.

But we already did that job for Gauss and confluent hypergeometric functions (A. Deaño, A. Gil, JS, JAT (2004))

For 100D accuracy, 3-4 iterations per root are enough and the method has proved reliability.

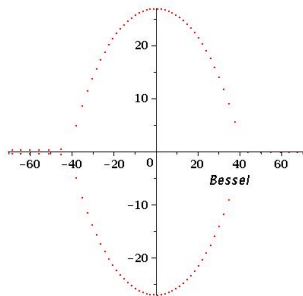


Computing complex zeros of special functions

The complex zeros of solutions of ODEs

$$y''(z) + A(z)y(z) = 0,$$

with $A(z)$ a complex meromorphic function, lie over certain curves.



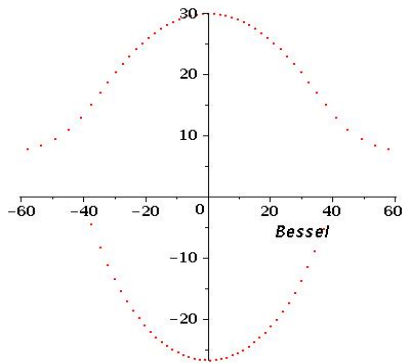
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$

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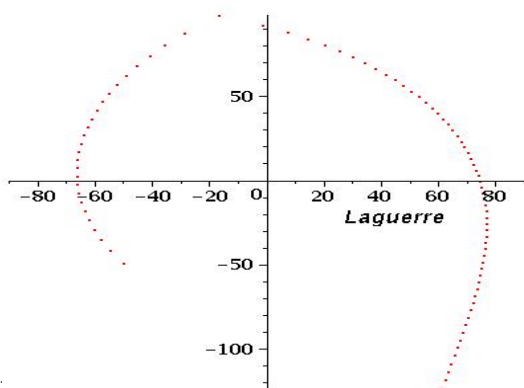
Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $z = 30i$.

Computing complex zeros of special functions

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Zeros of $L_n^{(\alpha)}(z)$, $n = 26.2$, $\alpha = -83 + 20i$

Which are those curves?

Consider that two independent solutions of the ODE in a domain D can be written as

$$y_{\pm}(z) = q(z)^{-1/2} \exp(\pm iw(z)), \quad w(z) = \int^z q(\zeta) d\zeta$$

If $y(z)$ is a solution such that $y(z^{(0)}) = 0$ then

$$y(z) = Cq(z)^{-1/2} \sin\left(\int_{z^{(0)}}^z q(\zeta) d\zeta\right)$$

Considering the parametric curve $z(\lambda)$, with $z(0) = z^{(0)}$ and satisfying

$$q(z(\lambda)) \frac{dz}{d\lambda} = 1$$

then $z(k\pi)$ are zeros of $y(z)$ because $\int_{z^{(0)}}^{z(k\pi)} q(\zeta) d\zeta = k\pi$, $k \in \mathbb{Z}$.

Therefore, we have zeros over the integral curve (an exact anti-Stokes line)

$$\frac{dy}{dx} = -\tan(\phi(x, y)), \quad q(z) = |q(z)| e^{i\phi(x, y)} \quad (2)$$

passing through $z(0) = x(0) + iy(0)$



Problem: for computing $q(z)$ we need to solve

$$\frac{1}{2}q(z)\frac{d^2q(z)}{dz^2} - \frac{3}{4}\left(\frac{dq(z)}{dz}\right)^2 - q(z)^4 - A(z)q(z)^2 = 0$$

which seems worse than our original problem, which was solving

$$y''(z) + A(z)y(z) = 0.$$

A drastic simplification

If $A(z)$ is constant the general solution of $y''(z) + A(z)y(z) = 0$ is

$$y(z) = C \sin(\sqrt{A(z)}(z - \psi)),$$

and the zeros are over the line

$$z = \psi + e^{-i\frac{\varphi}{2}} \lambda, \lambda \in \mathbb{R}, \varphi = \arg A(z)$$

The zeros lie over the integral lines

$$\frac{dy}{dx} = -\tan(\varphi/2). \quad (3)$$

Ansatz: the zeros are approximately over (3) even if $A(z)$ is not a constant.

This approximation is equivalent to consider $q(z) \approx \sqrt{A(z)}$. This is the WKB (or Liouville-Green) approximation:

$$y(z) \approx CA(z)^{-1/4} \sin\left(\int_{z(0)}^z A(\zeta)^{1/2} d\zeta\right)$$



A Sturm-like result for the WKB approximation

Let $z^{(0)}$, $z^{(1)}$ be consecutive zeros of the WKB approximation over an approximate anti-Stokes line (ASL). Then

$$\int_{z^{(0)}}^{z^{(1)}} A(\zeta)^{1/2} d\zeta = \pm\pi$$

And if $|A(z^{(0)})| > |A(z)|$ over the ASL between both zeros

$$L > \frac{\pi}{\sqrt{|A(z^{(0)})|}}$$

with L the length of the ASL arc. This is a Sturm-like result for the WKB approx.

If $A(z)$ has slow variation and $\Re z^{(1)} > \Re z^{(0)}$

$$z^{(1)} \approx z_1 = z^{(0)} + \frac{\pi}{\sqrt{A(z^{(0)})}}$$

First step towards an algorithm:

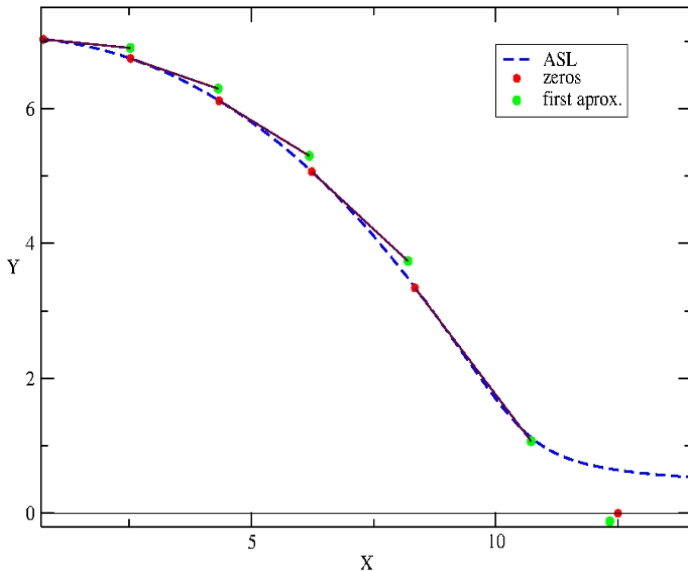
Let $z^{(0)}$ such that $y(z^{(0)}) = 0$. If $|A(z)|$ decreases for increasing $\Re z$ the next zero can be computed as follows:

$$\textcircled{1} \quad z_0 = H^+(z^{(0)}) = z^{(0)} + \pi / \sqrt{A(z^{(0)})}$$

$\textcircled{2}$ Iterate $z_{n+1} = T(z_n)$ until $|z_{n+1} - z_n| / |z_n| < \epsilon$, with

$$T(z) = z - \frac{1}{\sqrt{A(z)}} \arctan \left(\sqrt{A(z)} \frac{y(z)}{y'(z)} \right)$$

- a Step 1 depends on WKB and the fact that $A(z)$ has slow variation.
- b The straight line joining the points $y(z^{(0)})$ and $y(z_0)$ is tangent to the ASL arc at $z^{(0)}$. It is a **step in the right direction** and with an appropriate size if $A(z)$ varies slowly enough.
- c Step 2 is a fixed point method of order 4, independently of the WKB approx.

Numerical example for $Y_{10.35}(z)$.

Things to consider before constructing an algorithm:

- 1 Where to start the iterations for computing a first zero
- 2 How to choose the appropriate direction
- 3 When to stop
- 4 How many **ASLs** do we need to consider

It is important to determine the structure of anti-Stokes and Stokes lines.

Stokes line through z_0 : the curve

$$\Re \int_{z_0}^z \sqrt{A(\zeta)} d\zeta = 0,$$

Anti-Stokes line through z_0 : the curve

$$\Im \int_{z_0}^z \sqrt{A(\zeta)} d\zeta = 0.$$

Some properties:

- 1 If $z_0 \in \mathbb{C}$ is not a zero or a singularity of $A(z)$ there is one and only one ASL passing through that point. The same is true for the Stokes lines.
- 2 If z_0 is not a zero or a singularity of $A(z)$ the ASL and the SL passing through that point intersect perpendicularly at z_0 .
- 3 If z_0 is a zero of $A(z)$ of multiplicity m , $m + 2$ ASLs (and SLs) emerge from z_0

Studying the ASLs and SLs for

$$y''(z) + az^{-m}y(z) = 0,$$

we see that indeed $m + 2$ ASLs (and SLs) emerge from $z = 0$ if $m \neq 2$.

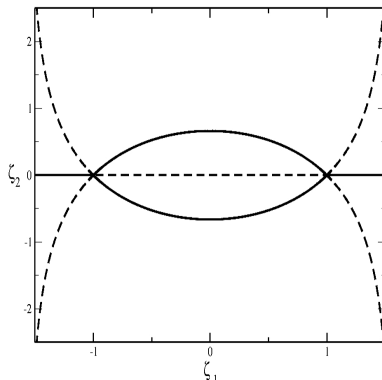
Example: Bessel functions

Principal (dashed line) and anti-Stokes (solid line) for the equation

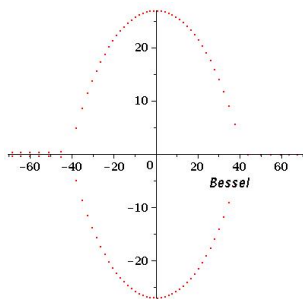
$$\frac{d^2 y}{d\zeta^2} + (1 - \zeta^{-2})y = 0$$

(Bessel equation of orders $|\nu| > 1/2$ with the change $z = \zeta\sqrt{\nu^2 - 1/2}$).

Principal lines of $y''(z) + A(z)y(z) = 0$ are those emerging from the zeros of $A(z)$.

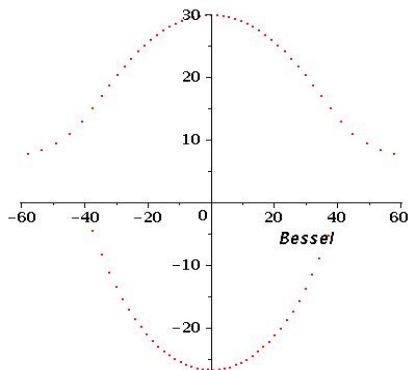


This explains the different patterns of zeros shown before.



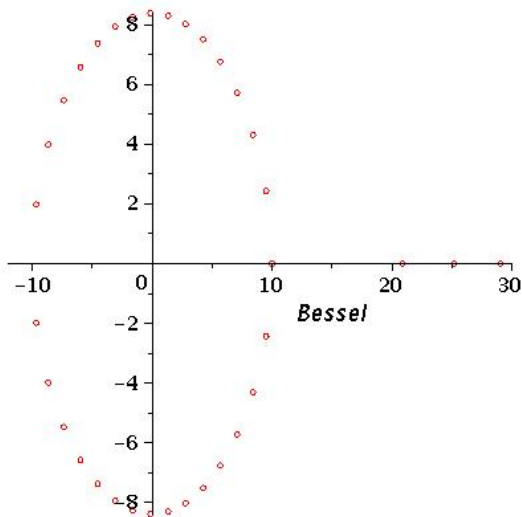
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$

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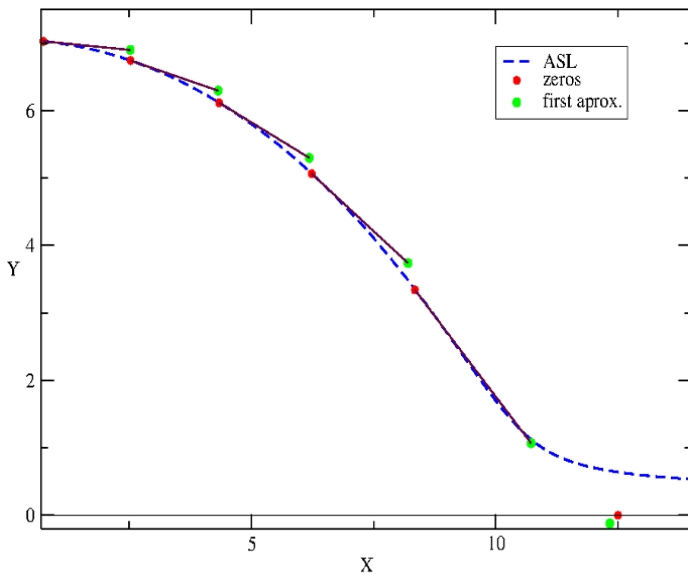


Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $30i$.

This explains the different patterns of zeros shown before.



Zeros of the Bessel function of order $\nu = 15.8$ and with a zero at $z = 10$.



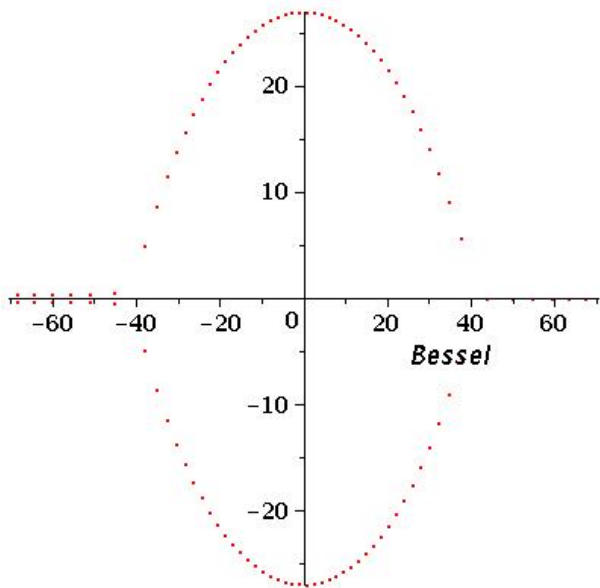
The strategy combines the use of $H^{(\pm)} = z \pm \frac{\pi}{\sqrt{A(z)}}$ and

$T(z) = z + \frac{1}{\sqrt{A(z)}} \arctan \left(\sqrt{A(z)} \frac{y(z)}{y'(z)} \right)$, following these rules:

- 1 Divide the complex plane in disjoint domains separated by the principal ASLs and SLs and compute separately in each domain.
- 2 In each domain, start away of the principal SLs, close to a principal ASL and/or singularity (if any). Iterate $T(z)$ until a first zero is found. If a value outside the domain is reached, stop the search in that domain.
- 3 Proceed with the basic algorithm, choosing the displacements $H^{(\pm)}(z)$ in the direction of approach to the principal SLs and/or singularity.
- 4 Stop when a value outside the domain is reached.

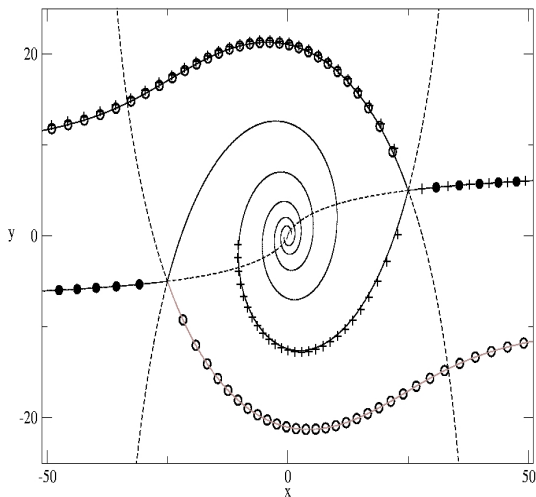
No exception has been found (so far tested for Bessel functions, PCFs and Bessel polynomials). See JS, Numerische Mathematik, to appear.
The method has fourth order convergence.

We finish with some graphical examples, with zeros computed using our algorithm in Maple.

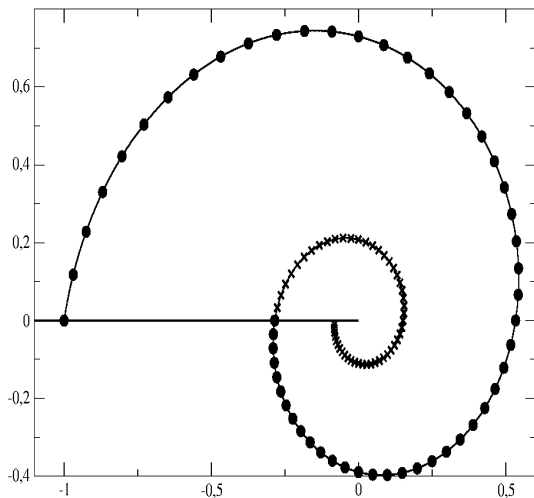


Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40:35$

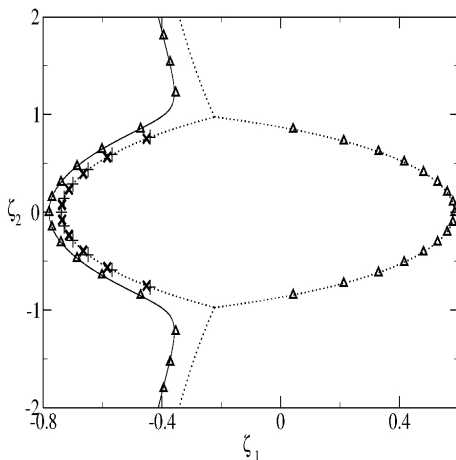




Stokes and anti-Stokes lines for the Bessel equation of order $\nu = 25 + 5i$, together with the zeros of $Y_\nu(x)$ (+), $J_\nu(x)$ (•) and $J_{-\nu}(x)$ (o).



Zeros of the two Bessel functions $y_\nu^{(k)} = e^{i\phi_k} \alpha J_\nu(z) + e^{-i\phi_k} \beta J_{-\nu}(z)$, $\phi_k = 2\nu k\pi$, $\mathbf{k} = \mathbf{0}, -1$, with α and β such that $y_\nu^{(0)}(-1 + 0^+i) = 0$. $\nu = 25 + 5i$.



Zeros of the Bessel polynomials $L_n^{(1-2n-a)}(2z)$ in the variable $\zeta = z/|\gamma|$, $|\gamma| = \sqrt{(n+a/2)(n+a/2-1)}$. All the cases shown share the same ASLs and SLs in the variable ζ . The symbols \times and $+$ correspond to the polynomial solutions $n = 10$, $a = 8$ and $n = 11$, $a = 8.572394\dots$. Triangles correspond to the non-polynomial case $n = 10.6$, $a = 8.343446\dots$.

THANK YOU!