Evaluación numérica de ceros de funciones especiales

Javier Segura

Universidad de Cantabria

RSME 2013, Santiago de Compostela

1. **Introduction**

2. **Fast and reliable computation of the real zeros of SFs**
   - The global method as a consequence of Sturm comparison
   - Examples

3. **Fast computation of the complex 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.

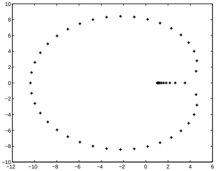
Efficiency: the total count of iterations is small (and if the order of convergence is high so much the better).

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,...).

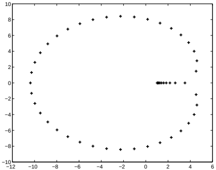
1. Special functions satisfy certain properties and equations (DDEs, TTRRs, ODEs,...)

1. Special functions satisfy certain properties and equations (DDEs, TTRRs, ODEs,...)
2. The zeros form regular patterns. Examples:

1. Special functions satisfy certain properties and equations (DDEs, TTRRs, ODEs,...)
2. The zeros form regular patterns. Examples:
   1. Zeros of classical orthogonal polynomials: real and in the interval of orthogonality.
   2. Even for non-classical cases, regular patterns occur:



1. Special functions satisfy certain properties and equations (DDEs, TTRRs, ODEs,...)
2. The zeros form regular patterns. Examples:
   1. Zeros of classical orthogonal polynomials: real and in the interval of orthogonality.
   2. Even for non-classical cases, regular patterns occur:



   3. Interlacing of the zeros of neighbour functions (example: positive zeros of the Bessel functions $J_\nu(x)$ and $J_{\nu\pm 1}(x)$).
3. In some cases, analytic approximations are available

Most published algorithms rely on first approximations + Newton method.

Reliable?: certainly not (no proof of convergence).

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

Additionally, one needs particular approximations for each different function.
They become difficult to handle for functions depending on several parameters (say Jacobi polynomials).

Not only the method matters, but also the function.
For computing zeros of solutions of

$$w''(x) + B(x)w'(x) + C(x)w(x) = 0 \tag{1}$$

using the Newton method we have order 2 generally, but if $C(x)$ is differentiable and $B(x) = 0$ the order is 3.
Assuming that $B(x)$ is differentiable 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 $A(x) = C(x) - \frac{1}{2}B'(x) - \frac{1}{4}B(x)^2$ and

$$\frac{y(x)}{y'(x)} = \frac{w(x)}{\frac{1}{2}B'(x)w(x) + w(x)}$$

The Newton method $x_{n+1} = x_n - \dfrac{y(x)}{y'(x)}$ is now of third order.

If a function satisfies a differential equation it is a good idea to use their coefficients.

If a function satisfies a differential equation it is a good idea to use their coefficients.

We have used just one coefficient. But we still have another one...

Construction of a fixed point method of order 4

Taking $h(x)=y(x)/y'(x)$, and because $y''(x)+A(x)y(x)=0$:
$h'(x)=1+A(x)h(x)^2$.

Construction of a fixed point method of order 4

Taking $h(x) = y(x)/y'(x)$, and because $y''(x) + A(x)y(x) = 0$:
$h'(x) = 1 + A(x)h(x)^2$.
If $y(\alpha) = 0$ and $A(x)$ has slow variation:

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

Construction of a fixed point method of order 4

Taking $h(x) = y(x)/y'(x)$, and because $y''(x) + A(x)y(x) = 0$:
$h'(x) = 1 + A(x)h(x)^2$.
If $y(\alpha) = 0$ and $A(x)$ has slow variation:

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

and assuming $A(x) > 0$

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

Order of convergence

A classroom exercise:

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

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

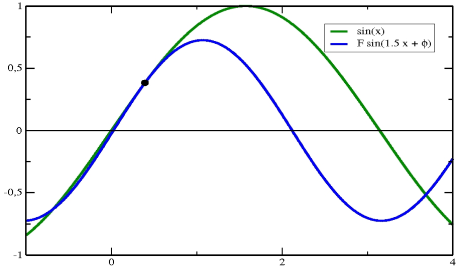
with $y''(x) + A(x)y(x) = 0$ and $A(x)$ differentiable has order four.

Direct computation shows that, if $y(\alpha) = 0$, then

$$g'(\alpha) = g''(\alpha) = g'''(\alpha) = 0,\ g^{(4)}(\alpha) = 2A'(\alpha)$$

Theorem (Sturm comparison)

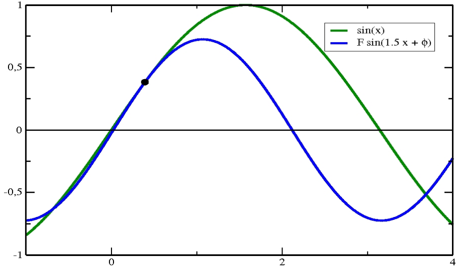
Let $y(x)$ and $w(x)$ be solutions of $y''(x) + A_y(x)y(x) = 0$ and $w''(x) + A_w(x)w(x) = 0$ respectively, with $A_y(x) > A_w(x) > 0$. If $y(x_0)w'(x_0) - y'(x_0)w(x_0) = 0$ and x_y and x_w are the zeros of $y(x)$ and $w(x)$ closest to x_0 and larger (or smaller) than x_0, then $x_y < x_w$ (or $x_y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



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.



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

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

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

$$T(x) = x - \frac{1}{\sqrt{A(x)}}\mathrm{arctan}_j(\sqrt{A(x)}h(x))$$

with

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

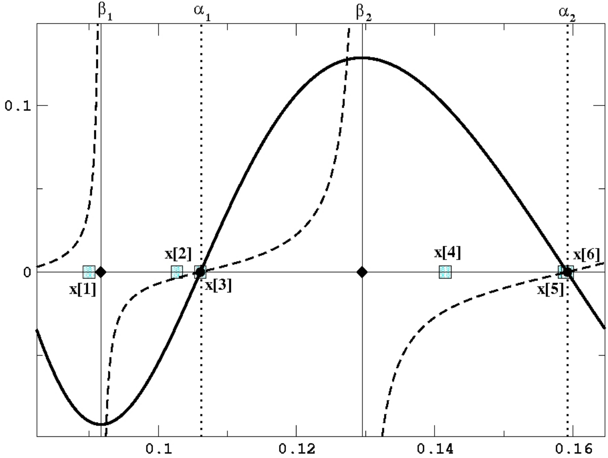
This method converges to α for any x_0 in $[\alpha', \alpha)$ if $A'(x) < 0$, with α' the largest zero smaller than α (analogously for $A'(x) > 0$).

The method has fourth order convergence:

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

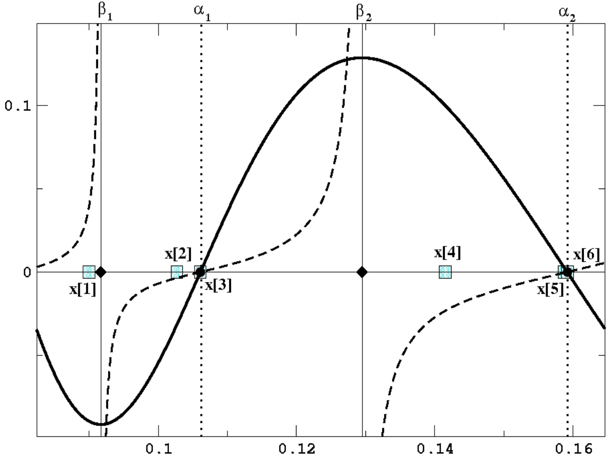
Computing the zeros in an interval where $A(x)$ is monotonic.

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.

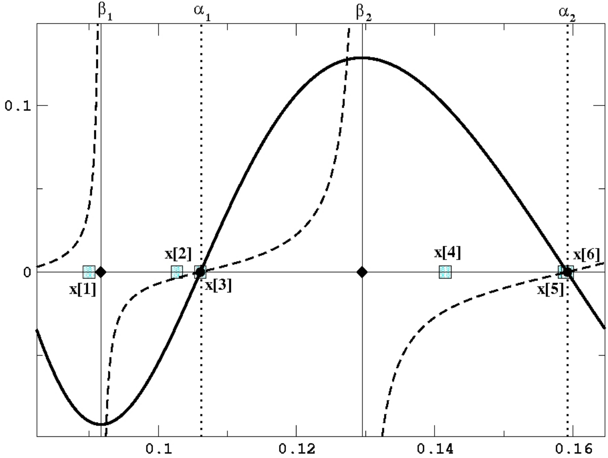
Example: zeros of $y(x) = x\sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



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.

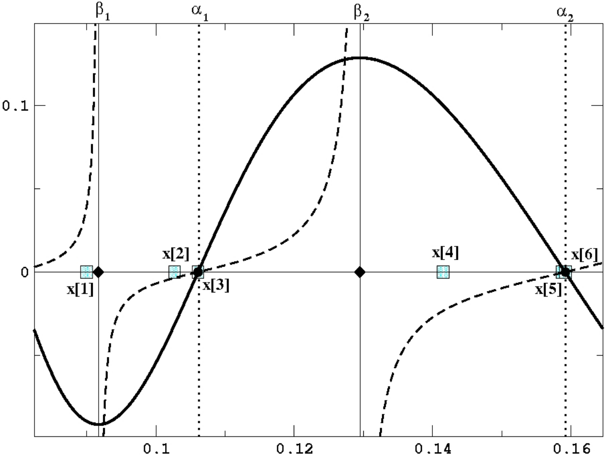
Example: zeros of $y(x) = x\sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



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

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. $x[4] = x[3] + \pi/A(x[3])$ (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).

Features of the method

1. Faster than Newton-Raphson (order 4), and globally convergent.
2. No initial guesses for the roots needed.
3. Computes with certainty all the roots in an interval, without missing any one.
4. **Good non-local behavior** and low total count of iterations
5. For 100D accuracy, 3-4 iterations per root are enough.

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

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

1. Confluent hypergeometric functions
    1. Laguerre functions (including Laguerre polynomials)
    2. Parabolic cylinder functions (including Hermite polynomials)
    3. Bessel functions of real or imaginary order and variable.
    4. Coulomb functions
2. Gauss hypergeometric functions
    1. Jacobi functions (including Jacobi, Gegenbauer and Legendre polynomials)
    2. Associated Legendre functions and conical functions.

The monotonicity of $A(x)$ is obtained by simply solving quadratic equations (with convenient Liouville transformations of the ODE)

In other cases, computing the regions of monotony may be not so straightforward. An example is provided by the zeros of

$$x\mathcal{C}_\nu + \gamma\mathcal{C}_\nu'(x)$$

with $\mathcal{C}_\nu(x)$ solutions of the Bessel equation

$$x^2 y''(x) + xy'(x) + (x^2 - \nu^2)y(x) = 0.$$

For computing these zeros, we first obtain the second order ODE satisfied by $\tilde{y}(x) = y'(x)$. Transform to normal form with a change of function. Solve the monotonicity and then apply the fourth order method.

Studying of the monotonicity of the resulting coefficient $A(x)$ implies solving cubic equations. (already done by Martin Muldoon, 1984)

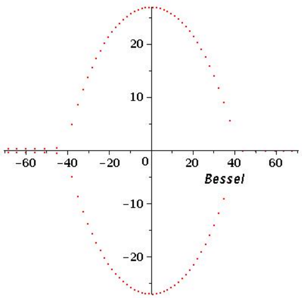
The resulting method is fast and reliable, also for the computation of double zeros (A. Gil, JS, Comput Math. Appl. (2012)).

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.



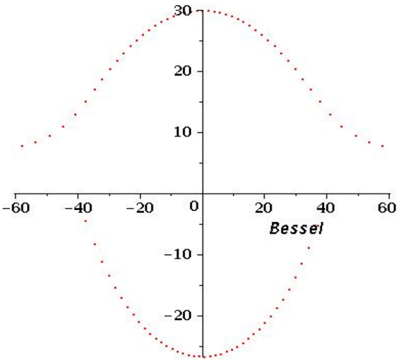
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$

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.



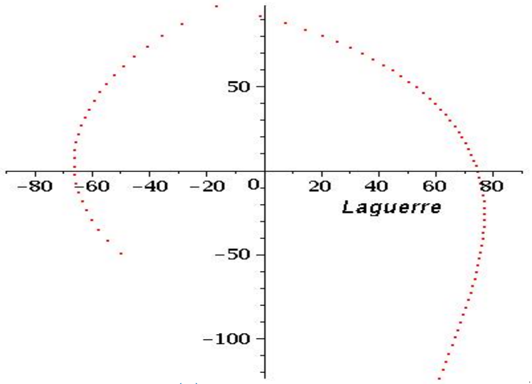
Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $z = 30i$.

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

Which are those curves?

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

$$y_{\pm}(z) = q(z)^{-1/2} \exp\left(\pm i w(z)\right), \; w(z) = \int^{z} q(\zeta) d\zeta$$

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

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

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 $\displaystyle\int_{z(0)}^{z(k\pi)} q(\zeta) d\zeta = k\pi$, $k \in \mathbb{Z}$.

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

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

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:

1. $z_0=H^{+}(z^{(0)})=z^{(0)}+\pi/\sqrt{A(z^{(0)})}$
2. Iterate $z_{n+1}=T(z_n)$ until $|z_{n+1}-z_n|<\epsilon$, with

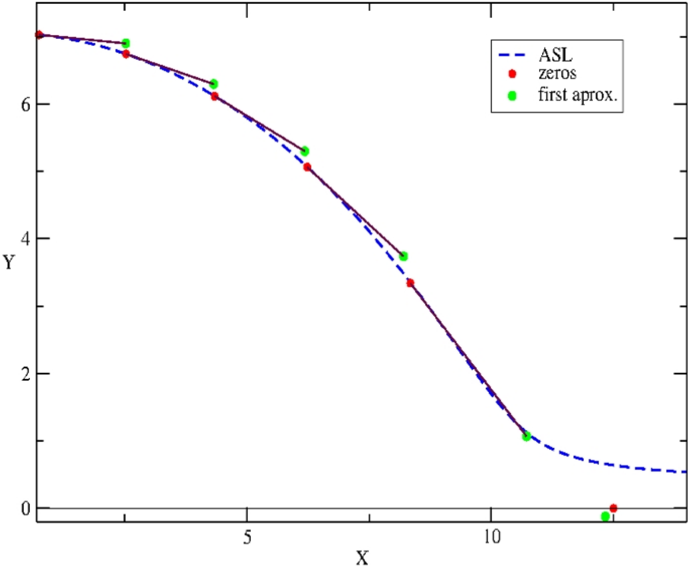
$$T(z)=z-\frac{1}{\sqrt{A(z)}}\arctan\left(\sqrt{A(z)}\frac{y(z)}{y'(z)}\right)$$

a Step 1 depends on WKB and the fact that $A(z)$ has slow variation.

b The straight line joining the points y $z^{(0)}$ y z_0 is tangent to the ASL arc at $z^{(0)}$. It is a step in the right direction and with an appropiate 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, $m+2$ ALSs (and SLs) emerge from z_0

Studying the ASLs and SLs for

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

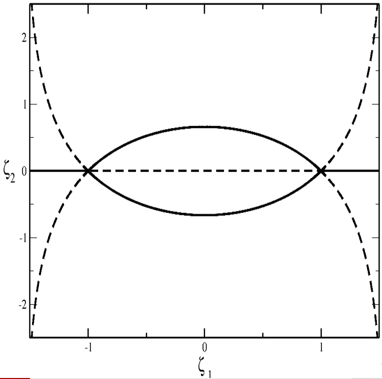
we see that indeed $m+2$ ASLs (and SLs) emerge from $z=0$ if $m \neq 2$.

Example: Bessel functions

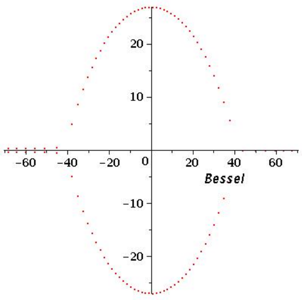
Principal (dashed line) and anti-Stokes (solid line) for the equation

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

(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 $A(z)$.

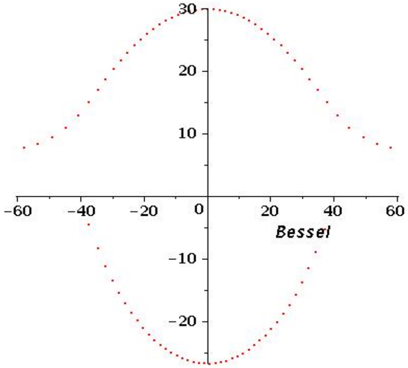


This explains the different patterns of zeros shown before.



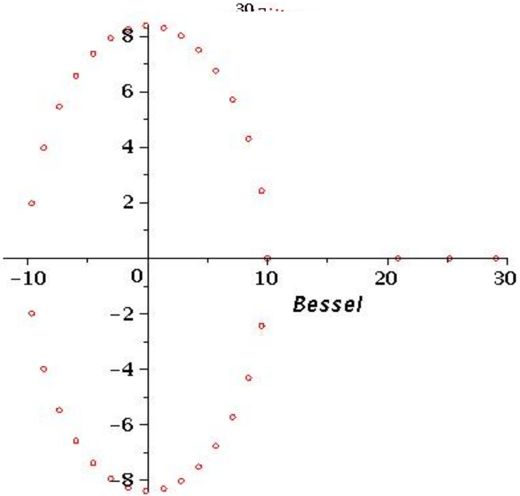
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$

This explains the different patterns of zeros shown before.

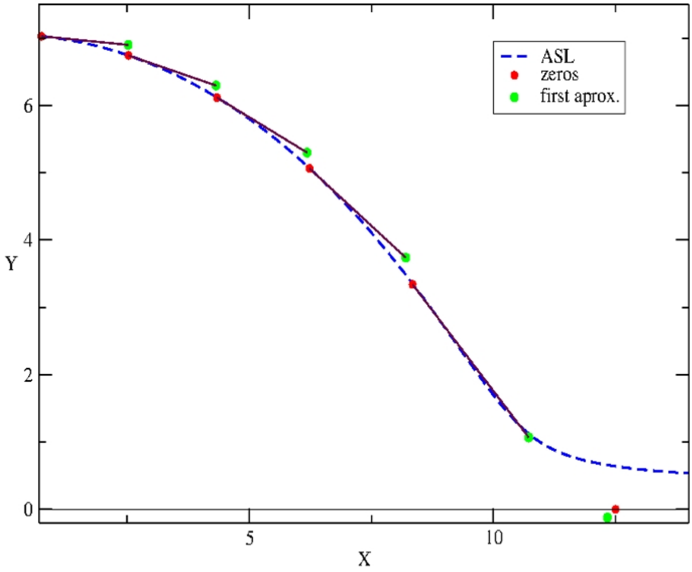


Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $30i$.

This explains the different patterns of zeros shown before.



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

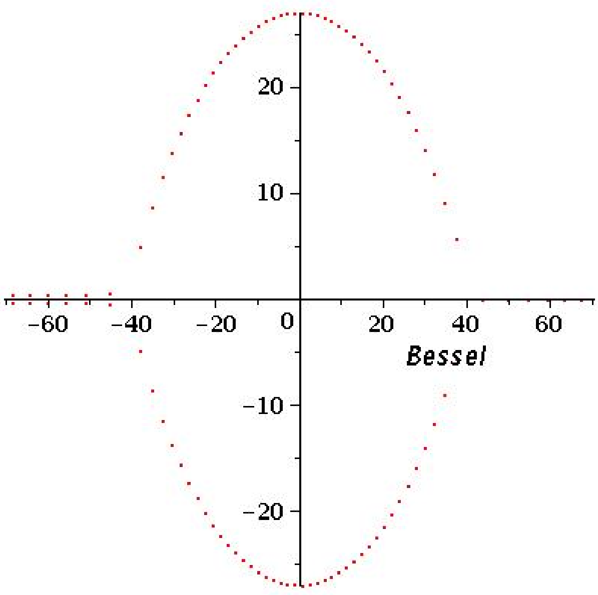

ASL
zeros
first aprox.
Y
X
0
2
4
6
5
10

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

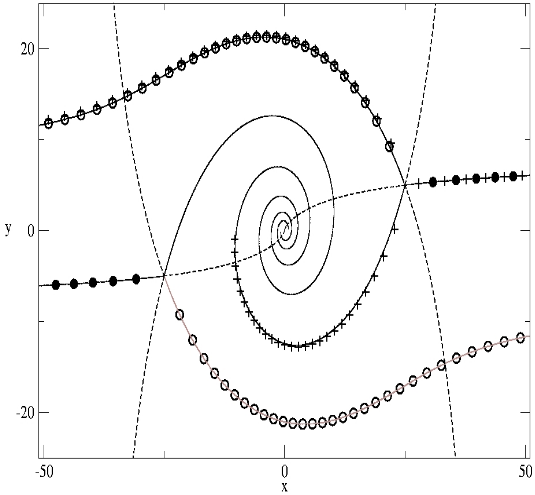
$T(z) = z + \dfrac{1}{\sqrt{A(z)}} \arctan\left(\sqrt{A(z)}\dfrac{y(z)}{y'(z)}\right)$, following these rules:

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.

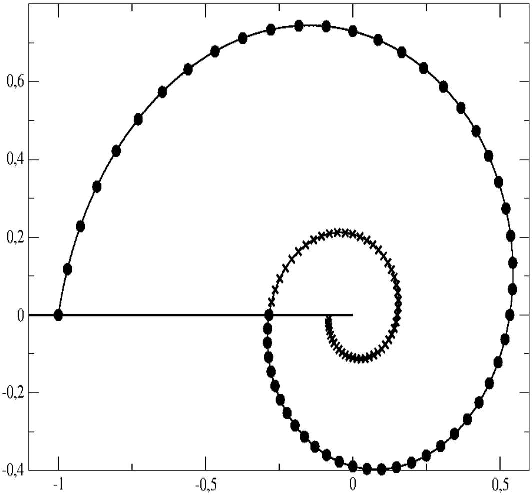
No exception has been found (so far tested for Bessel functions, PCFs and Bessel polynomials).
The method has fourth order convergence.



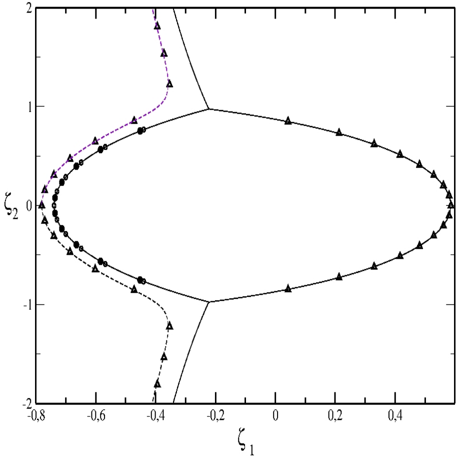
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$



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



Zeros of the two Bessel functions $y_\nu^{(k)} = e^{i\phi_k}\alpha J_\nu(z) + e^{-i\phi_k}\beta J_{-\nu}(z),\ \phi_k = 2\nu k\pi$, $\boldsymbol{k = 0, -1}$, 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. Black and white circles correspond to the polynomial solutions $n = 10$, $a = 8$ and $n = 11$, $a = 8.572394\ldots$ Triangles correspond to the non-polynomial case $n = 10.6$, $a = 8.343446..$

For finishing:

Conjecture

The zeros of the generalized Bessel polynomials $\theta_n(z/\gamma, a)$ cluster over the curve

$$
\begin{array}{l}
|p(z)| = 1, \Re(z) < \cos\phi, \\
p(z) = e^{V(z)} \left(\dfrac{V(z) - z + \cos\phi}{\sin\phi} \right)^{\cos\phi} \dfrac{z \sin\phi}{1 - z\cos\phi + V(z)}, \\
V(z) = \sqrt{1 - 2z\cos\phi + z^2} \\
\cos\phi = (1 - a/2)/\gamma,\ \gamma = \sqrt{(n + a/2)(n + a/2 - 1)}
\end{array}
\tag{4}
$$

when $n \to \infty$, with a or a/n fixed.

The case $a = 2$ ($\cos\phi = 0$) gives a known result (Bruin, Saff & Varga 1981): a $n \to +\infty$ the zeros of $\theta_n(z/n; a) \equiv \theta_n(z/n)$ cluster over the curve $|q(z)| = 1$, $\Re z < 0$, where

$$
q(z) = \exp(\sqrt{z^2+1}) \frac{z}{1 + \sqrt{z^2+1}} \tag{5}
$$

THANK YOU!