Some analytical and numerical consequences of Sturm theorems

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1. **Sturm theorems and some applications (non-numerical)**
   - Sturm theorems for second order ODEs
   - First order differential systems (oscillatory case)
   - First order differential systems (monotonic case)
2. **Numerical applications: computing real zeros**
   - Methods for first order systems
   - A fourth order method for second order ODEs
3. **Complex zeros**

We consider second order ODEs $y''(x)+A(x)y(x)=0$ with $A(x)$ continuous in an interval.

Theorem (Sturm separation theorem)

Let y_1 and y_2 be independent solutions of $y''(x)+A(x)y(x)=0$, $A(x)>0$. Between two zeros of each solution there is a zero of the other solution and only one.

Theorem (Sturm comparison theorem (1^{st} version))

Let y_i, $i=1,2$, be solutions of $y_i''(x)+A_i(x)y_i(x)=0$, $i=1,2$ with $A_i(x)$ continuous and $0<A_1(x)\leq A_2(x)$ in an interval I.
Let $x_1,x_2\in I$ such that $y_1(x_1)=y_1(x_2)=0$. Then, there exist at least one value $c\in(x_1,x_2)$ such that $y_2(c)=0$ unless $y_1(x)=y_2(x)$.

Theorem (Spacing and convexity)

Let $y(x)$ be a non-trivial solution of $y'' + A(x)y = 0$. Let $x_k < x_{k+1} < \dots$ denote consecutive zeros of $y(x)$ arranged in increasing order.
Then

1. *If $A(x) \leq A_M$ in (x_k, x_{k+1}), $A_M > 0$, (but $A(x) \not\equiv A_M$) then*

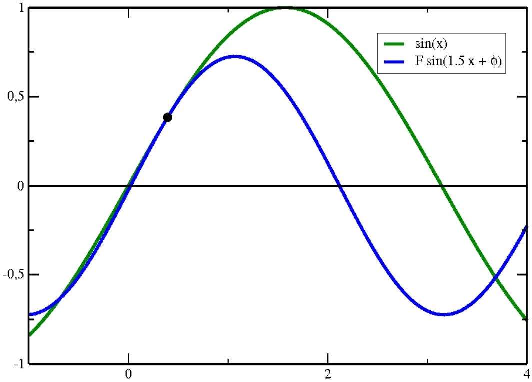
$$\Delta x_k \equiv x_{k+1} - x_k > \frac{\pi}{\sqrt{A_M}} .$$

2. *If $A(x) \geq A_m > 0$ in (x_k, x_{k+1}) (but $A(x) \not\equiv A_m$) then*

$$\Delta x_k \equiv x_{k+1} - x_k < \frac{\pi}{\sqrt{A_m}} .$$

3. *If $A(x)$ is strictly increasing in (x_k, x_{k+2}) then $\Delta^2 x_k \equiv x_{k+2} - 2x_{k+1} + x_k < 0$.*
4. *If $A(x)$ is strictly decreasing in (x_k, x_{k+2}) then $\Delta^2 x_k \equiv x_{k+2} - 2x_{k+1} + x_k > 0$.*

Main idea: the greater is the coefficient $A(x) > 0$ in the differential equation $y''(x) + A(x)y(x) = 0$, the more rapid is the oscillation, and the shorter the distance between zeros.



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

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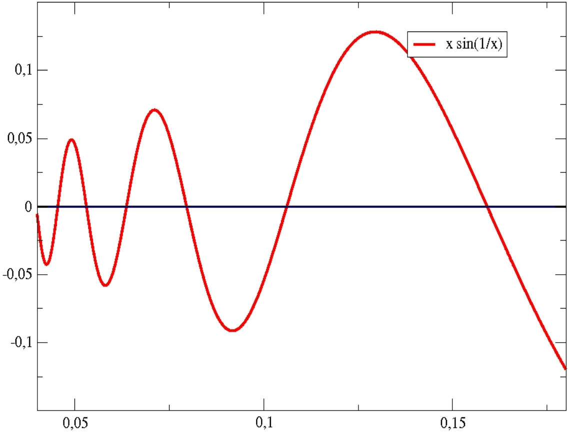


Equation: $y''(x) + x^{-4}y(x) = 0$

The Liouville transformation for ODEs

Given

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

then the function $Y(z)$, with $Y(z(x))$ given by

$$Y(z(x)) = \sqrt{z'(x)}\exp\left(\frac{1}{2}\int^{x} B(x)\right) y(x),$$

satisfies the equation in normal form

$$\ddot{Y}(z) + \Omega(z)Y(z) = 0$$

$$\Omega(z(x)) = \frac{1}{z'(x)^2}\left(\tilde{A}(x) + \frac{3z''(x)^2}{4z'(x)^2} - \frac{z'''(x)}{2z'(x)}\right),$$

$$\tilde{A}(x) = A(x) - B'(x)/2 - B(x)^2/4$$

Question (for hypergeometric functions): for which changes of variable is the analysis of the monotonicity of $\Omega(x)$ simple?

Simple: $\Omega'(x)=0$ equivalent to a quadratic equation.

1. $z'(x)=x^{p-1}(1-x)^{q-1}$; $p+q=1$ or $p=0$ or $q=0$ (Gauss hypergeometric)
2. $z'(x)=x^{p-1}$ (confluent)

Examples (Gauss):
$p=q=1/2$: bounds on $\Delta\theta_k$, θ_k the zeros of $P_n^{\alpha,\beta}(x)$ (Szegő-like)
$p=0$, $q=1$: $(1-x_k)^2>(1-x_{k+1})(1-x_{k-1})$, $|\alpha|\leq 1$ (Grosjean-like)
$p=1$, $q=0$: $(1+x_k)^2>(1+x_{k+1})(1+x_{k-1})$, $|\beta|\leq 1$
[A. Gil, A. Deaño, JS, **JAT** 2004]

Monotonic and oscillating systems

Consider a first order system

$$\begin{aligned} y'(x) &= a(x)y(x) + d(x)w(x) \\ w'(x) &= b(x)w(x) + e(x)y(x) \end{aligned}$$

Typical situation: $y = y_n$, $w = y_{n-1}$ and coefficients depending on n.
Defining $h(x) = y(x)/w(x)$, we have

$$h'(x) = d(x) - (b(x) - a(x))h(x) - e(x)h^2(x)$$

Given $\Delta(x) = (b(x) - a(x))^2 + 4e(x)d(x)$:

1. $\Delta < 0$ ($e(x)d(x) < 0$): potentially oscillatory $\Rightarrow$ Sturm
2. $\Delta > 0$ Monotonic $\Rightarrow$ "sturmish"

Theorem (Sturm separation theorem)

Let $y = y_n$ and $w = y_{n-1}$ be non-trivial continuous solutions of the first order system with $d(x)$ and $e(x)$ continuous and not changing sign. Then, the zeros of y_n and y_{n-1} are simple and they are **interlaced** *(between two zeros of each solution there is a zero of the other solutions and only one).*

A first result (same orthogonal sequence):

Theorem

Let $p_{n+1}(x)$ and $p_{n-1}(x)$ be two classical orthogonal polynomials (Hermite, Laguerre, Jacobi) with respect to the same weight function $w(x)$ in the interval of orthogonality $[a, b]$. Then, the zeros of $p_{n+1}(x)$ and $p_{n-1}(x)$ are interlaced for $x > \beta_n$ and $x < \beta_n$, with

$$\beta_n = \frac{\displaystyle\int_a^b x p_n^2(x) w(x) dx}{\displaystyle\int_a^b p_n^2(x) w(x) dx} \in (a, b)$$

If x_1 and x_2 are the closest zeros of $p_{n+1}(x)$ at both sides of β_n ($x_1 < \beta_n < x_2$) then, either there is no zero of $p_{n-1}(x)$ in (x_1, x_2) or $x = \beta_n$ is a common zero of $p_{n+1}(x)$ and $p_{n-1}(x)$.

Some other results (different orthogonal sequences)

Theorem

The zeros of $P_{\nu}^{(\alpha,\beta)}(x)$ *interlace with those of* $P_{\nu'}^{(\alpha',\beta')}(x)$ *in* $(-1,1)$ *if the differences* $\delta\nu=\nu-\nu'\in\mathbb{Z}$, $\delta\alpha=\alpha-\alpha'\in\mathbb{Z}$ *and* $\delta\beta=\beta-\beta'\in\mathbb{Z}$ *(not all of them equal to zero) satisfy simultaneously the following properties:*

1. $|\delta\nu|\leq 1$
2. $|\delta\alpha|+|\delta\beta|\leq 2$
3. $|\delta\nu+\delta\alpha|\leq 1$, $|\delta\nu+\delta\beta|\leq 1$, $|\delta\nu+\delta\alpha+\delta\beta|\leq 1$

This holds whenever $\nu>0$, $\nu+\alpha>0$ *and* $\nu+\beta>0$, $\nu+\alpha+\beta>0$ *and similarly for* ν', α' *and* β', *with the exception of the zeros for* $P_{\nu}^{(+1,\beta)}(x)$ *and* $P_{\nu+1}^{(-1,\beta)}(x)$ *which coincide in* $(-1,1)$; *the same is true for the zeros of* $P_{\nu}^{(\alpha,+1)}(x)$ *and* $P_{\nu+1}^{(\alpha,-1)}(x)$.

[JS, Numerical Algorithms (2008)]

Interlacing properties of the zeros of orthogonal polynomials have been studied by K. A. Driver and collaborators.

Sturm comparison for first order systems

From now on, we consider systems

$$\begin{aligned} y'(x) &= \eta(x)y(x) + w(x), \\ w'(x) &= -\eta(x)y(x) - y(x). \end{aligned}$$

and the associated Riccati equation for $h(x) = y(x)/w(x)$:

$$h'(x) = 1 - 2\eta(x)h(x) + h(x)^2$$

Transformation to reduced form

Given a general system with differentiable coefficients a, b, c and d as before, we take

$$\begin{aligned} \widetilde{y}(z(x)) &= \sqrt{\frac{z'(x)}{|d|}} \exp\left(-\frac{1}{2}\int^x (a+b)\right) y(x), \\ \widetilde{w}(z(x)) &= \sqrt{\frac{z'(x)}{|e|}} \exp\left(-\frac{1}{2}\int^x (a+b)\right) w(x) \end{aligned}$$

with $z'(x) = \sqrt{|d(x)e(x)|}$, and the transformed system takes the form

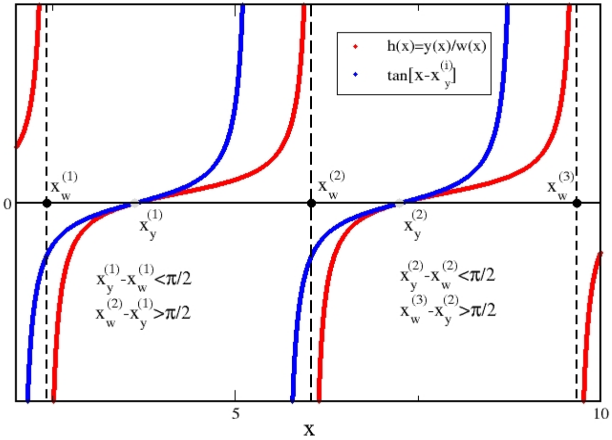
$$\begin{aligned} \dot{\widetilde{y}}(z) &= -\widetilde{\eta}(z)\widetilde{y}(z) + \widetilde{d}(z)w(z), \\ \dot{\widetilde{w}}(z) &= \widetilde{\eta}(z)\widetilde{w}(z) + \widetilde{e}(z)y(z), \\ |\widetilde{d}(z)| &= |\widetilde{e}(z)| = 1 \end{aligned}$$

with

$$\widetilde{\eta}(z) = \dot{x}\,\frac{b(z) - a(z)}{2} + \frac{1}{4}\frac{d}{dz}\log\left|\frac{d(z)}{e(z)}\right|$$

Sturm comparison

$h'(x)=1-2\eta(x)h(x)+h(x)^2, \quad 0<\eta(x)<1$



This is a starting point for the numerical method in [JS, SIAM J. Numer. Anal. (2002)]

Theorem (Sturm comparison)

Let $\{y(x), w(x)\}$ *solutions of a system in reduced form with* $0 < \eta_1 < \eta(x) < \eta_2 < 1$. *Let* x_y^i *and* $x_w^{(i)}$ *denote zeros of* y *and* w *such that* $x_w^{(1)} < x_y^{(1)} < x_w^{(2)}$ *then*

$$\frac{1}{\sqrt{1-\eta_2^2}} \arctan\left(\frac{\sqrt{1-\eta_2^2}}{\eta_2}\right) < x_y^{(1)} - x_w^{(1)} < \frac{1}{\sqrt{1-\eta_1^2}} \arctan\left(\frac{\sqrt{1-\eta_1^2}}{\eta_1}\right)$$

$$\frac{\pi}{2\sqrt{1-\eta_1^2}} < x_w^{(2)} - x_y^{(1)} < \frac{\pi}{2\sqrt{1-\eta_2^2}}$$

Theorem (Sturm convexity)

Let $\{y(x), w(x)\}$ *as before and with* $0 < \eta(x) < 1$, $\eta'(x) > 0$. *Let* $x_w^{(1)} < x_y^{(1)} < x_w^{(2)} < x_y^{(2)} < x_w^{(3)}$ *then*

$$x_y^{(1)} - x_w^{(1)} > x_y^{(2)} - x_w^{(2)}$$

and

$$x_w^{(2)} - x_y^{(1)} < x_w^{(3)} - x_y^{(2)}$$

Bounds for monotonic differential systems

By the moment, let us consider the case $d(x)e(x) > 0$.

A first example (modified Bessel functions) [JS, JMAA 2011]:
$y_\nu = e^{i\pi\nu}K_\nu(x)$ and $I_\nu(x)$ satisfy

$$y_\nu'(x) = -\frac{\nu}{x}y_\nu(x) + y_{\nu-1}(x),$$

$$y_{\nu-1}'(x) = \frac{\nu-1}{x}y_{\nu-1}(x) + y_\nu(x),$$

And from this,

$$y_{\nu+1}(x) + \frac{2\nu}{x}y_\nu(x) - y_{\nu-1}(x) = 0 \quad (TTRR),$$

$$x^2 y_\nu''(x) + xy_\nu' - (x^2+\nu^2)y_\nu(x) = 0 \quad (ODE)$$

and

$$h_\nu'(x) = 1 - \frac{2\nu-1}{x}h_\nu(x) - h_\nu(x)^2,\ h_\nu(x) = y_\nu(x)/y_{\nu-1}(x)$$

A bound for first kind MBFs:

Solving $h'_\nu(x)=0$ ($h'_\nu(x)=y_\nu(x)/y_{\nu-1}(x)$) we see that

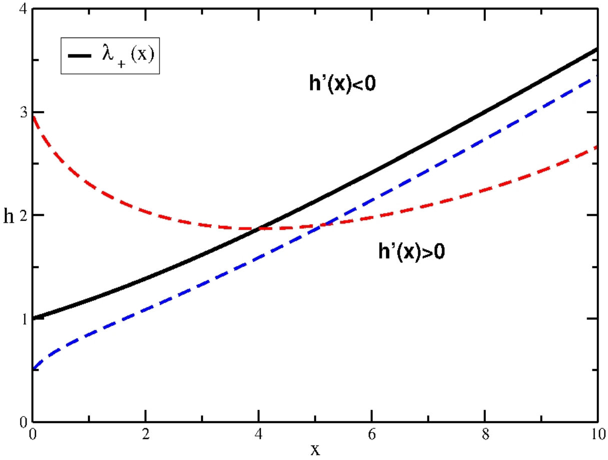
1. $h'_\nu(x)<0$ if $h_\nu(x)>\lambda_\nu^+(x)$
2. $h'_\nu(x)>0$ if $0<h_\nu(x)<\lambda_\nu^+(x)$

$$\lambda_\nu^+(x)=x/(\nu-1/2+\sqrt{(\nu-1/2)^2+x^2})$$

But because $h_\nu(x)=I_\nu(x)/I_{\nu-1}(x)$ is such that $h_\nu(0^+)>0$ and $h'_\nu(0^+)>0$ ($\nu\geq 0$) and $\boldsymbol{d\lambda_\nu^+/dx>0}$ if $\nu\geq 1/2$, then, necessarily:

$$0<\frac{I_\nu(x)}{I_{\nu-1}(x)}<\lambda_\nu^+(x),\ x>0,\ \nu\geq 1/2$$

The situation is described in the next graph (blue curve):



More general case

[JS, J. Ineq. Appl. 2012]

$$\begin{aligned} y_n'(x) &= a_n(x)y_n(x) + d_n(x)y_{n-1}(x) \\ y_{n-1}'(x) &= b_n(x)y_{n-1}(x) + e_n(x)y_n(x) \end{aligned}$$

We will consider the case $e_n(x)d_n(x) > 0$

$$h_n'(x) = d_n(x) - (b_n(x) - a_n(x))h_n(x) - e_n(x)h_n(x)^2$$

We have $h_n'(x) = 0$ when $h_n(x) = \lambda_n^{\pm}(x)$ and the following holds

Monotonicity of the roots

Let $y_k(x)$, $k = n, n-1$ satisfying

$$\begin{aligned} y_n'(x) &= a_n(x)y_n(x) + d_n(x)y_{n-1}(x), \\ y_{n-1}'(x) &= b_n(x)y_{n-1}(x) + e_n(x)y_n(x) \end{aligned}$$

with $d_n(x)e_n(x) > 0$ and $y_k''(x) + B(x)y_k'(x) + A_k(x)y_k(x) = 0$. Then, if $A_n(x) \neq A_{n-1}(x)$, the characteristic roots $\lambda_n^{\pm}(x)$ are monotonic in (a, b). $d\lambda_n^{\pm}(x)/dx$ have the same sign as $A_{n-1}(x) - A_n(x)$ and $-\eta_n'(x)$.

$$\begin{array}{l} y'(x) = a(x)y(x) + d(x)w(x), \\ w'(x) = b(x)w(x) + e(x)y(x) \end{array} , \; h(x) = y(x)/w(x)$$

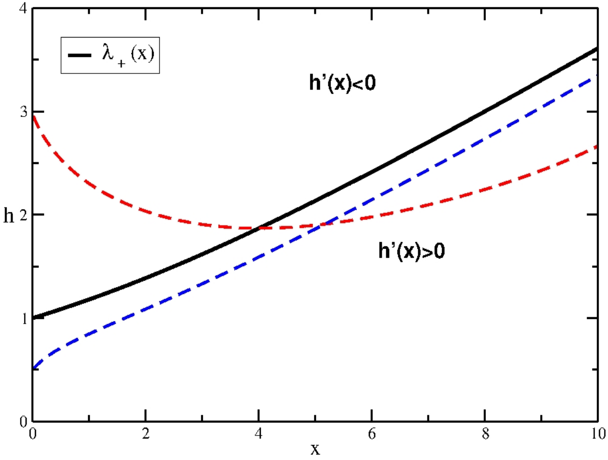
We take $d(x) > 0$, $e(x) > 0$ ($\lambda_+ > 0$ and $\lambda_- < 0$)

Lemma (Bounds for the case $h(a^+) > 0$)

- *If $h(a^+) > 0$, $\lambda_+(x)$ is monotonic and $h'(a^+)\lambda_+'(a^+) > 0$ (or, equivalently, $(h(a^+) - \lambda_+(a^+))\lambda_+'(a^+) < 0$) then $(h(x) - \lambda_+(x))\lambda_+'(x) < 0$ in (a, b).*
- *If $h(a^+) > 0$, $\lambda_+(x)$ is monotonic and $h'(a^+)\lambda_+'(a^+) < 0$ then either $h(x)$ reaches one relative extremum at $x_e \in (a, b)$ (a minimum if $\lambda_+'(x) > 0$ and a maximum if $\lambda_+'(x) < 0$) or $(h(x) - \lambda_+(x))\lambda_+'(x) > 0$ in (a, b).*

The case $h(b^-) < 0$ is analogous but with respect to λ_-.

Bounds in an interval (a, b). Case $h(a^+) > 0$



Bounds and the asymptotics of the TTRR

$$e_{n+1}y_{n+1}(x)+(b_{n+1}(x)-a_n(x))y_n(x)-d_ny_{n-1}(x)=0,$$

Characteristic roots: $e_{n+1}\bar{\lambda}_n^2+(b_{n+1}-a_n)\bar{\lambda}_n-d_n=0,$

Theorem (Perron-Kreuser)

If $\lim_{n\to+\infty}|\bar{\lambda}_n^{(+)}/\bar{\lambda}_n^{(-)}|\neq 1$ *solutions* $\{y_k^{(1)},y_k^{(2)}\}$ *exist such that*

$$\lim_{n\to+\infty}\frac{1}{\bar{\lambda}_n^{+}}\frac{y_n^{(1)}}{y_{n-1}^{(1)}}=1,\ \lim_{n\to+\infty}\frac{1}{\bar{\lambda}_n^{-}}\frac{y_n^{(2)}}{y_{n-1}^{(2)}}=1.$$

Charac. roots of Riccati equation: $e_n\lambda_n^2+(b_n-a_n)\lambda_n-d_n=0.$

Consequence: as $n\to\infty$ the bounds tend to be sharper.

Iteration of the TTRR

The TTRR can be used to generate sequences of bounds (convergent sequences for minimal solutions of TTRR).

For instance, if $b_{n+1} - a_n$ and $y_{n+1}/y_n > 0$ the solution is minimal and with the backward iteration

$$\frac{y_n(x)}{y_{n-1}(x)} = d_n \left(b_{n+1} - a_n + e_{n+1} \frac{y_{n+1}(x)}{y_n(x)} \right)^{-1}$$

sequences of upper and lower bounds are obtained.
This gives additional Perron-Kreuser bounds.

Forward iteration gives sequences of bounds for dominant solutions.

From the upper and lower bounds: Turán-type inequalities.

$$l_n = \min_x (L_n(x)) < L_n(x) < \frac{y_n}{y_{n+1}} \frac{y_n}{y_{n-1}} < U_n(x) < \max_x (U_n(x)) = u_n$$

Using the differential system: bounds on logarithmic derivatives

LG bounds

Under appropriate conditions the following holds if $d\lambda_n^s/dx > 0$, $s = sign(y_n(x)/y_{n-1}(x))$:

$$s\frac{y'_{n-1}(x)}{y_{n-1}(x)} < s\frac{a_n(x)+b_n(x)}{2} + \sqrt{d_n(x)e_n(x)}\sqrt{1+\eta_n(x)^2} < s\frac{y'_n(x)}{y_n(x)}$$

If $d\lambda_n^s/dx < 0$ the inequalities are reversed

1. Modified Bessel functions

Bounds for $I_\nu(x)$, $K_\nu(x)$, as well as new Turán-type inequalities, like for, instance

$$\frac{K_{\nu-1}(x)}{K_\nu(x)}\frac{K_{\nu+1}(x)}{K_\nu(x)} < \frac{|\nu|}{|\nu|-1},\ x>0,\ \nu\notin[-1,1]$$

Used in the literature (related to a parameter of a probablity distribution) without proof [JS, JMAA (2011)]
[Baricz, Bull. Aust. Math. Soc (2010)]
See also Laforgia and Natalini, J. Inequal. Appl. (2010)

2. Parabolic cylinder functions, solutions of $y'' - (x^2/4+n)y = 0$, $a>0$. $h_n(x) = -U(n,x)/U(n-1,x)$, $h_n(0+)<0$

For $n>1/2$ and $x\geq 0$ the following holds

$$2\left(x+\sqrt{4n+2+x^2}\right)^{-1} < \frac{U(n,x)}{U(n-1,x)} < 2\left(x+\sqrt{4n-2+x^2}\right)^{-1}$$

The lower bound also holds if $n\in(-1/2,1/2)$ and this inequality turns to an equality if $n=-1/2$.

Turán-type inequalities for PCFs

Let $F(x) = \dfrac{U(n,x)^2}{U(n-1,x)U(n+1,x)}$.
The following holds for all real x:

$$\sqrt{\frac{n-3/2}{n+1/2}} < \frac{n-1/2}{n+1/2}F(x) < 1 < F(x) < \sqrt{\frac{n+3/2}{n-1/2}}$$

The first inequality holds for $n>3/2$ and the rest for $n>1/2$. For $x<0$ the third inequality also holds if $n\in(-1/2,1/2)$.

Baricz & Ismail also considered related inequalities recently (Const. Aprox. (2012))

LG bounds for PCFs

For all real x and $n \geq 1/2$ the following holds:

$$-\sqrt{x^2/4+n+1/2} < \frac{U'(n,x)}{U(n,x)} < -\sqrt{x^2/4+n-1/2}$$

The left inequality also holds for $n > -1/2$.

Consequence of the previous inequality

$$B_{n+1/2}(x) < \frac{U(a,x)}{U(a,0)} < B_{n-1/2}(x)$$

where

$$B_\alpha(x) = \exp\left(-\frac{x}{2}\sqrt{\frac{x^2}{4}+\alpha}\right)\left(\frac{x}{2\sqrt{\alpha}}+\sqrt{\frac{x^2}{4\alpha}+1}\right)^{-\alpha}$$

Some Turán-type inequalities for OPs

$$H_n(ix)^2 - \sqrt{(n-1)/(n+1)}H_{n-1}(ix)H_{n+1}(ix) > 0,\ n \text{ even.}$$

3. Associated Legendre functions of imaginary variable

$$\frac{P_n^m(ix)^2}{P_{n-1}^m(ix)P_{n+1}^m(ix)} < 1 + \frac{1}{n-m},\ n-m \text{ odd}$$

4. Laguerre functions

For any $\nu \geq 0$ and $\alpha \geq 0$, $x > 0$ the following holds:

$$\frac{\nu}{\nu+1}\frac{\alpha}{\alpha+1} < \frac{L_{\nu+1}^{\alpha-1}(-x)}{L_\nu^\alpha(-x)}\frac{L_{\nu-1}^{\alpha+1}(-x)}{L_\nu^\alpha(-x)} < \frac{\nu}{\nu+1}$$

Case $d_n(x)e_n(x) < 0$ (an example)

○ Hermite polynomials $x \in \mathbb{R}$.

$$\frac{H_n(x)}{H_{n-1}(x)} > x + \sqrt{x^2 - 2(n-1)}, x > \sqrt{2(n-1)}$$

Therefore, the largest zero of $H_n(x)$ is smaller than $\sqrt{2(n-1)}$ if $n > 1$

Two iterations with the recurrence relation give:

Theorem

The largest zero of $H_n(x)$ is smaller than $\sqrt{2(n-2)}$ if $n > 2$ and smaller than $\sqrt{2(n-3)}$ if $n > 6$

(The bounds in Dimitrov, Nikolov, JAT(2010) are slightly better)
Continuing with the iterations: $\sqrt{2n-12}$ is an upper bound for $n \geq 39$ (but asymptotics is more powerful for large n, see Elbert, Muldoon, Contemp. Math (2008))

Numerical applications: computation of zeros

The Sturm separation and comparison theorems for first order systems can be used to construct globally convergent fixed point methods for computing zeros of special functions.

These are (like Newton) second order methods but with the advantage that a scheme to compute with certainty all the zeros in an interval becomes available (JS, SIAM J Numer Anal, 2002). Global third order methods are also possible, but

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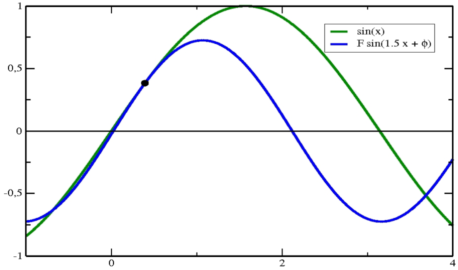
we move to the recent and more powerful fourth order methods based on Sturm theorems for second order ODEs.

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 $x_y>x_w$).



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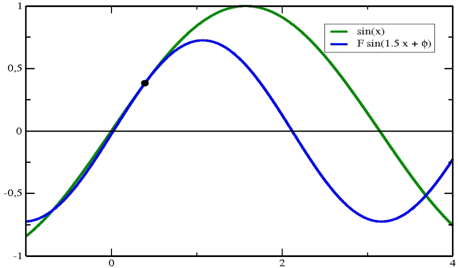


Algorithm (Zeros of $y''(x)+A(x)y(x)=0$, $A(x)$ monotonic)

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.

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

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

with

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

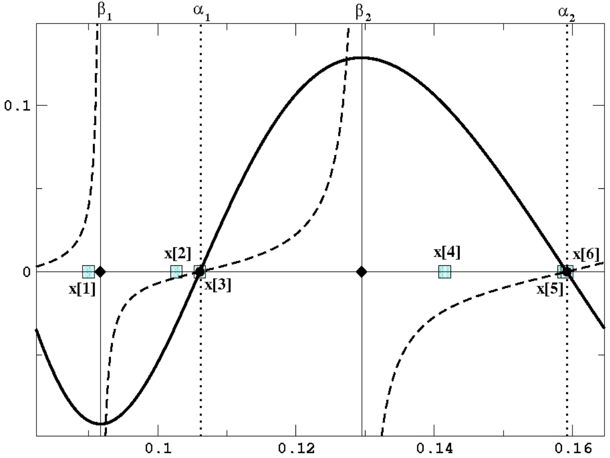
This method converges to α for any x_0 in $[\alpha', \alpha)$ if $A'(x) < 0$, with α' the largest zero smaller than α (analogously for $A'(x) > 0$).

The method has fourth order convergence:

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

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.).



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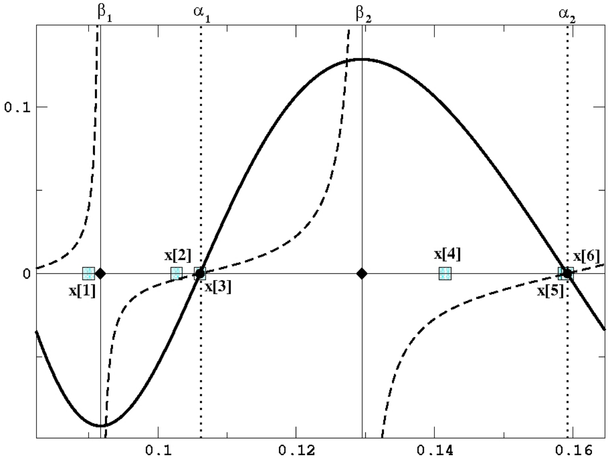

1. $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)

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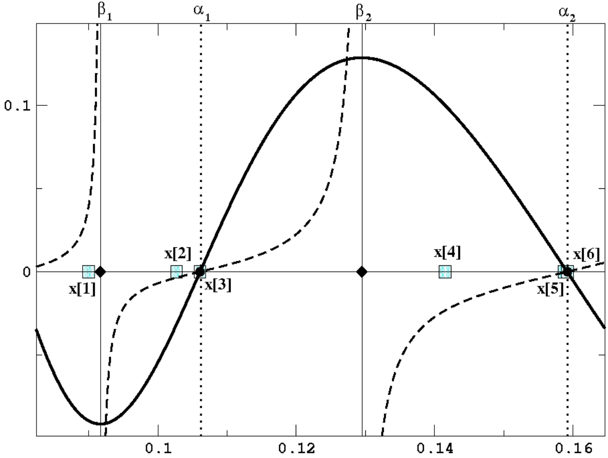

1. $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)
2. $x[4] = x[3] + \pi/A(x[3])$ (smaller than the next zero by Sturm comparison)

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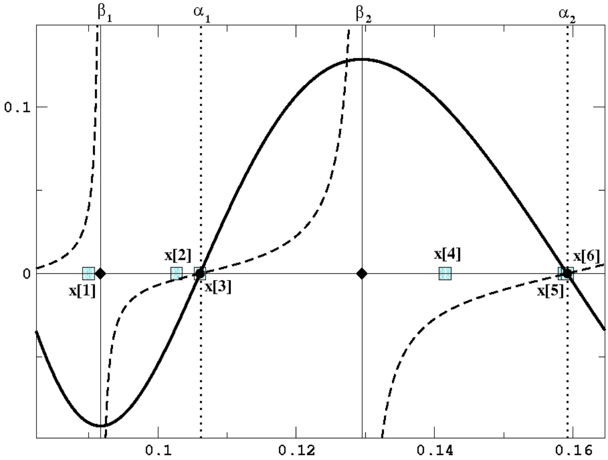

1. $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)
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3. $T(x[4]) = x[5]$, $T(x[5]) = x[6]$ (with four digits acc.)

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!

Other examples:

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

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

   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 (see M. Muldoon, Archivum Mathematicum (1982)).

   The resulting method is very efficient (order 4) and is reliable, also for the computation of double zeros (A. Gil, JS, Comput Math. Appl. (2012)).

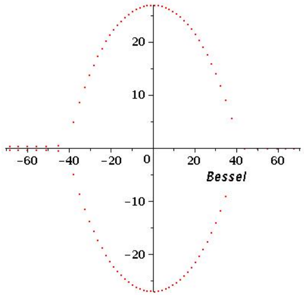
2. Fixed point methods $T(x) = x - w(x)^{-1} \arctan(w(x)y(x)/y'(x))$ are regularized Newton methods of local frequency $w(x)$. They can be applied to other functions, not necessarily solutions of ODEs. Example: cross products of Bessel functions.

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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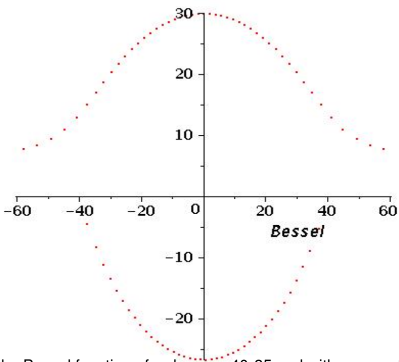

Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $z = 30i$.

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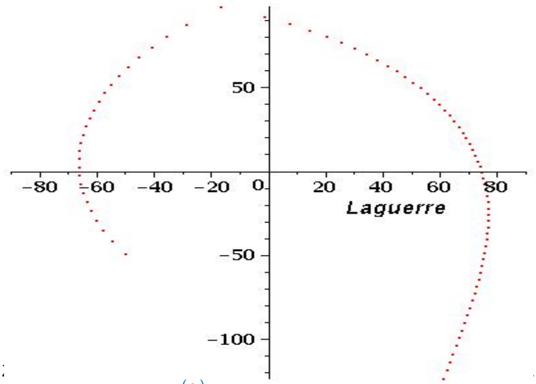


Zeros of $L_n^{(\alpha)}(z)$, $n = 26.2$, $\alpha = -83 + 20i$

Which are those curves?

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

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

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

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

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

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

$$\frac{dy}{dx}=-\tan(\phi(x,y)),\; q(z)=|q(z)|e^{i\phi(x,y)} \qquad (1)$$

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

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

Ansatz: the zeros are approximately over (2) even if $A(z)$ is not a constant. This approximation is equivalent to consider $q(z)\approx\sqrt{A(z)}$. This is the WKB 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

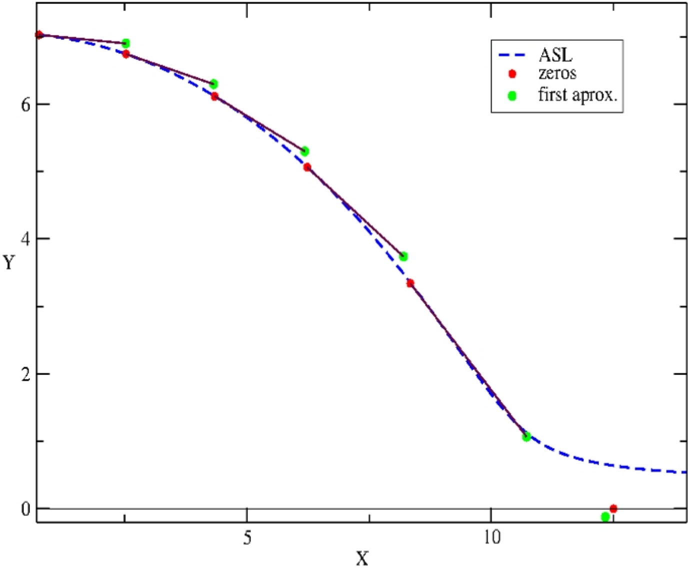
$$T(z) = z - \frac{1}{\sqrt{A(z)}} \arctan\left(\sqrt{A(z)}\frac{y(z)}{y'(z)}\right)$$

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

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

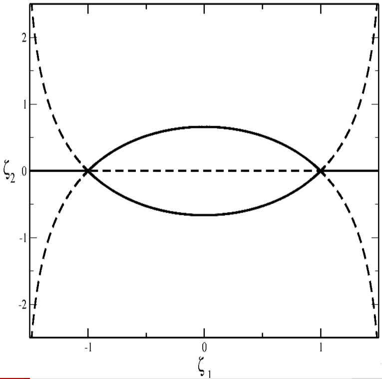
we see that indeed $m+2$ ASLs (and SLs) emerge from $z=0$ if $m \neq 2$.

Example: Bessel functions

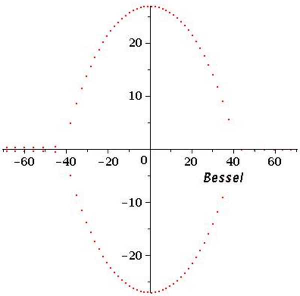
Principal (dashed line) and anti-Stokes (solid line) for the equation

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

(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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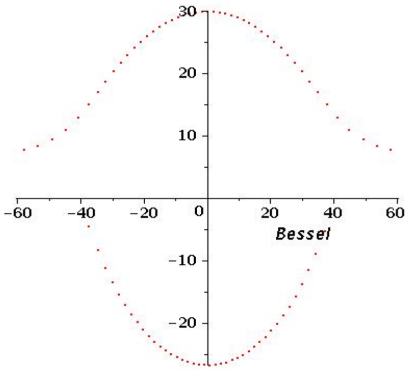

Zeros of the Bessel function of order $\nu = 40.35$ and with a zero at $30i$.

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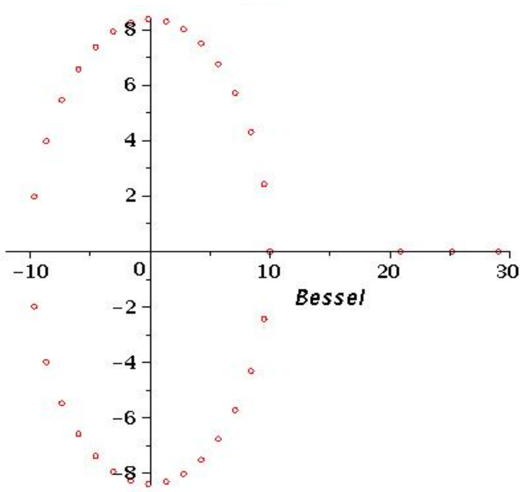
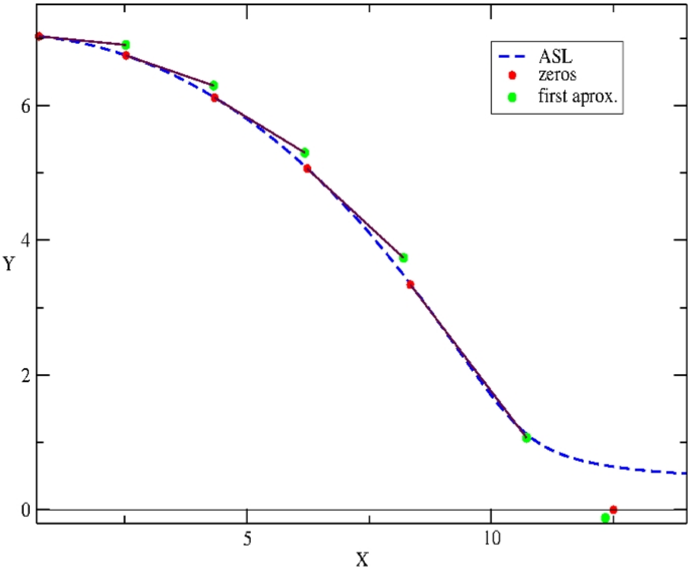


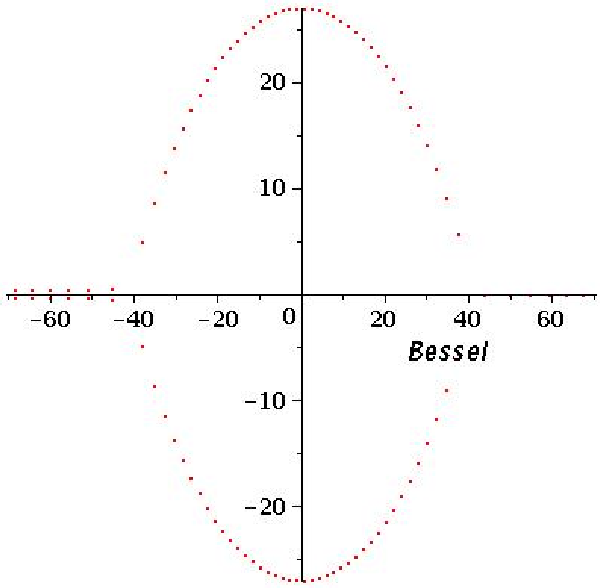
Zeros of the Bessel function of order $\nu = 15.8$ and with a zero at $z = 10$.


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

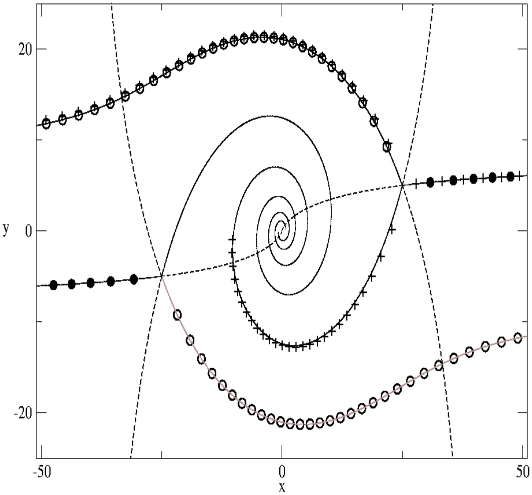
The stategy combines the use of $H^{(\pm)} = z \pm \frac{\pi}{\sqrt{A(z)}}$ and $T(z) = z + \frac{1}{\sqrt{A(z)}} \arctan\left(\sqrt{A(z)}\frac{y(z)}{y'(z)}\right)$, following these rules:

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.

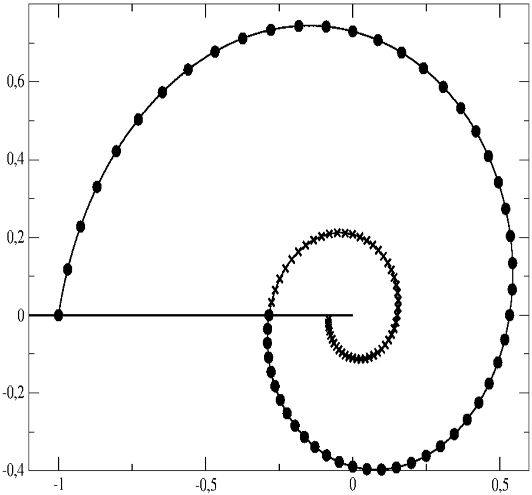
No exception has been found (so far tested for Bessel functions, PCFs and Bessel polynomials).
The method has fourth order convergence.



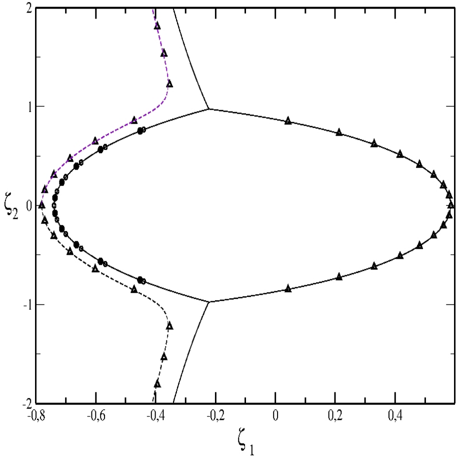
Zeros of the Bessel function $Y_\nu(z)$ of order $\nu = 40.35$



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

$$\begin{aligned} & |p(z)| = 1, \Re(z) < \cos\phi, \\ & p(z) = e^{V(z)} \left(\frac{V(z) - z + \cos\phi}{\sin\phi} \right)^{\cos\phi} \frac{z\sin\phi}{1 - z\cos\phi + V(z)}, \\ & V(z) = \sqrt{1 - 2z\cos\phi + z^2} \\ & \cos\phi = (1 - a/2)/\gamma,\ \gamma = \sqrt{(n + a/2)(n + a/2 - 1)} \end{aligned} \tag{3}$$

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

$$q(z) = \exp(\sqrt{z^2 + 1}) \frac{z}{1 + \sqrt{z^2 + 1}} \tag{4}$$

THANK YOU!