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Some Analytical and Numerical Consequences of Sturm Theorems

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Abstract

The Sturm comparison theorems for second order ODEs are classical results from which information on the properties of the zeros of special functions can be obtained. Sturm separation and comparison theorems are also available for difference-differential systems under oscillatory conditions. The separation theorem provides interlacing information for zeros of some special functions and the comparison theorem gives bounds on the distance between these interlacing zeros. For monotonic systems Sturm theorems for the zeros do not exist because there is one zero at most. Instead, bounds on certain function ratios can be obtained using information on the coefficients of the system, and particularly monotonicity properties. Similar ideas that can be used to prove Sturm theorems can be considered for obtaining this type of bounds; the qualitative analysis of associated Riccati equations is a key ingredient in both cases. We review some applications for modified Bessel, parabolic cylinder and Laguerre functions and we also present related results for incomplete gamma functions. Sturm theorems, both for second order ODEs and first order DDEs can be applied for the computation of the real zeros of special functions. Recently a fourth order method based on the Sturm comparison theorem for computing the real zeros of solutions of second order ODEs was developed. We discuss the connection of this method with the Sturm theorem and we explain how this has been extended to the computation of complex zeros.

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1 Introduction

Sturm theorems for linear homogeneous second order ordinary differential (ODEs) are classical results from which a good number of properties for the zeros of special functions have been established; see for instance [2, 10, 21]. Sturm separation and comparison theorems are also available for the difference-differential equations (DDEs)

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

under oscillatory conditions ($d_n(x)e_n(x) < 0$). The separation theorem provides interlacing information for zeros of some special functions and, in particular, for zeros of orthogonal polynomials belonging to different orthogonal sequences [15]. We provide a brief account of the results that we obtained both from the Sturm theorems for ODEs [2, 3, 14] and DDEs [13, 15].

For nonoscillatory situations ($(b_n(x) - a_n(x))^2 + 4d_n(x)e_n(x) > 0$) Sturm theorems for the zeros do not exist because there is one zero at most. In its place, it is possible to obtain bounds for the solutions; similar ideas that can be used to prove Sturm comparison theorems can be used for obtaining such bounds. Indeed, as we will see, most of these results can be obtained by studying the qualitative properties of associated Riccati equations. For this reason, we may consider that these are also, in some sense, results of Sturm type. We overview some of the results presented in [17, 18] and provide a new example (incomplete gamma function).

Much more recent is the application of Sturm theorems as numerical tools for solving some notable nonlinear equations (zeros of solutions of second order ODEs). The idea behind these methods, first introduced in [16], is to use the information on the speed of oscillation contained in the coefficient $A(x)$ of the differential equation $y''(x) + A(x)y(x) = 0$ in order to make estimations of the zeros. We briefly describe some particular applications for the real case as well as the extension to the complex plane introduced in [19].

2 Sturm Theorems for Second Order ODEs

We consider second order ODEs

$$y''(x) + A(x)y(x) = 0, A(x) > 0 \tag{2.1}$$

with $A(x)$ continuous in an interval. The following are two classical results appearing in textbooks.

Theorem 2.1 (Sturm separation theorem)**.** *Let y_1 and y_2 be independent solutions of* (2.1). *Then, between two zeros of each solution there is a zero of the other solution and only one.*

Theorem 2.2 (Sturm comparison theorem (1st 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 $y_1(x) = y_2(x)$.

A simple explanation of the previous theorem and the next one is that the solutions of a differential equation (2.1) oscillate more rapidly as $A(x)$ is larger. In particular, if for instance $A(x) < A_M$, the solutions of $y''(x) + A_M y(x) = 0$ oscillate more rapidly than the solutions of (2.1) and then the distance between to consecutive zeros of (2.1) will be larger than $\pi/\sqrt{A_M}$. Considering these type of arguments, the following results are easy to understand.

Theorem 2.3 (Spacing and convexity). *Let $y(x)$ be a nontrivial solution of $y''+A(x)y = 0$. Let $x_k < x_{k+1} < \ldots$ 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 not $A(x) = A_M \, \forall x \in (x_k, x_{k+1})$) 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 not $A(x) = A_m \, \forall x \in (x_k, x_{k+1})$) 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 $\Delta^2 x_k \equiv x_{k+2} - 2x_{k+1} + x_k > 0$.*

The two last results are again a consequence of the fact that has $A(x)$ becomes larger the oscillations are faster. Then, for instance, if $A(x)$ is increasing the oscillations are faster as x increases and if we have three consecutive zeros $x_k < x_{k+1} < x_{k+2}$ then $x_{k+2} - x_{k+1} < x_{k+1} - x_k$.

In Section 5 we will use a slightly more general version of the Sturm comparison theorem

Theorem 2.4 (Sturm comparison (2nd version)). *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 $A_w(x) > A_y(x) > 0$. 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 $x_w < x_y$ (or $x_w > x_y$).*

A proof can be formulated in terms of the associated Riccati equations; in fact, a similar proof can be considered for a more general result:

Theorem 2.5 (Sturm comparison (3rd version))**.** *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 $A_w(x) > A_y(x) > 0$ and such that $y(x_0)w'(x_0) - y'(x_0)w(x_0) = 0$. Given a value $x_y > x_0$ (or $x_y < x_0$) let $x_w \neq x_0$ be the closest value to x_0 larger (or smaller) than x_0 and such that $y(x_y)w'(x_w) - y'(x_y)w(x_w) = 0$, then $x_w < x_y$ (or $x_w > x_y$); therefore $|x_w - x_0| < |x_y - x_0|$.*

Proof. Let us consider the functions $h_y = y/y'$ and $h_w = w/w'$, satisfying the Riccati equations $h_y'(x) = 1 + A_y(x)h_y(x)^2$, $h_w'(x) = 1 + A_w(x)h_w(x)^2$. Because we are considering $A_y > 0$, $A_w > 0$, the h_y and h_w functions, assuming they have several zeros, are tangent–like functions with zeros (zeros of $y(x)$ or $w(x)$) and singularities (zeros of $y'(x)$ or $w'(x)$) interlaced. We assume that $y'(x_0) \neq 0$ and $w'(x_0) \neq 0$ (but it is immediate to see that the result is also valid in this case) and let us consider $x_y > x_0$ (the proof for $x_y < x_0$ is analogous).

Because $h_y(x_0) = h_w(x_0)$ and, given that $A_w > A_y$, $h_w'(x_0) > h_y'(x_0)$, and the graph of $h_w(x)$ lies above the graph of $h_y(x)$ at the right of x_0, and it keeps being above until it reaches its first vertical asymptote. Therefore, the function h_w reaches any value in the interval $(h_w(x_0), +\infty)$ before h_y does. This tangent–like functions change sign at its asymptotes and then, because $h_w'(x_c) > h_y'(x_c)$ for any x_c such that $h_w(x_c) \geq h_y(x_c)$, it is also clear that h_w also reaches any value between in the interval $(-\infty, h_w(x_0))$ before h_y does. Therefore, given any $x_y > x_0$ because for $x > x_0$ h_w reaches any value before h_y does it is clear that there exists $x_0 < x_w < x_y$ such that $h_w(x_w) = h_y(x_y)$. This completes the proof. □

Later we will consider proofs with a similar flavour for obtaining other results, not related to zeros of solutions of ODEs. In this sense, the bounds in Section 4 have a "Sturm flavour" even when they can not be considered Sturm theorems.

2.1 New Inequalities from Classical Sturm Theorems

The name of this section is the title of our paper [2]. In that paper, we proposed a systematic analysis of the results that theorem 2.3 can provide for the zeros of hypergeometric functions (Gauss, Kummer). In that analysis, it was crucial to take into account the freedom we have in the selection of the independent variable via the Liouville transformation.

As it is easy to check, given an ODE

$$y'' + B(x)y' + A(x)y = 0, \tag{2.2}$$

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

$$Y(z(x)) = \sqrt{z'(x)}\exp\left(\frac{1}{2}\int^x B(x)\right) y(x), \tag{2.3}$$

satisfies the equation in normal form

$$\ddot{Y}(z) + \Omega(z)Y(z) = 0 \tag{2.4}$$

$$\begin{aligned} \Omega(z(x)) &= \frac{1}{z'(x)^2}\left(\tilde{A}(x) + \frac{3z''(x)^2}{4z'(x)^2} - \frac{z'''(x)}{2z'(x)}\right) \\ \tilde{A}(x) &= A(x) - B'(x)/2 - B(x)^2/4. \end{aligned} \tag{2.5}$$

Using these transformations (called Liouville transformations) we can establish bounds on the distances between zeros and/or convexity properties, provided the analysis of the monotonicity properties of $\Omega(x)$ can be carried out. The main question that was considered in [2] was: for which changes of variable is the analysis of the monotonicity of $\Omega(x)$ simple in the sense that $\Omega'(x) = 0$ is equivalent to a quadratic equation? And the answer is:

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 hypergeometric equation).

The analysis, particularly for values of $p, q = 0, 1/2, 1$, provided extensions of known properties as well as new properties. We mention few examples for the case of Jacobi functions $P_\nu^{\alpha,\beta}(x)$ (polynomials if ν is a positive integer):

1. $p = q = 1/2$: Bounds on $\Delta\theta_k$, with θ_k the zeros of $P_\nu^{\alpha,\beta}(\cos\theta)$ were established which generalize and improve previous results by Szegő [21].
2. $p = 0$, $q = 1$: The relation $(1-x_k)^2 > (1-x_{k+1})(1-x_{k-1})$, was proved for the zeros of $|\alpha| \leq 1$ $P_\nu^{\alpha,\beta}(x)$, extending the previously known property for Legendre polynomials [9].
3. $p = 1$, $q = 0$: The relation $(1+x_k)^2 > (1+x_{k+1})(1+x_{k-1})$, is proved to be valid for $|\beta| \leq 1$.

The information on the monotonicity properties of $\Omega(x)$ is not only useful for establishing new Sturm properties for the zeros but, as we will see in Section 5, this is a crucial piece of information for the recent numerical methods for computing these zeros [16].

3 Sturm Theorems for First Order Differential Systems

Many special functions satisfy first order systems of the type

$$\begin{aligned} y'(x) &= a(x)y(x) + d(x)w(x), \\ w'(x) &= b(x)w(x) + e(x)y(x). \end{aligned} \tag{3.1}$$

A typical situation is when $y = y_n$, $w = y_{n-1}$ with n a parameter (for example, the degree in case of orthogonal polynomials) and with coefficients depending on n. In particular Gauss and Kummer hypergeometric functions satisfy this type of systems.

3.1 Monotonic and Oscillatory Systems

As we did for proving theorem 2.5, we are considering qualitative properties of an associated Riccati equation to explore properties of the solutions of the system (3.1).

Defining $h(x) = y(x)/w(x)$, we have the Riccati equation

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

The behavior of the solutions is different depending on whether the equation $d(x) - (b(x) - a(x))\lambda(x) - e(x)\lambda(x)^2 = 0$ has real or complex solutions. Depending on $\Delta(x) = (b(x) - a(x))^2 + 4e(x)d(x)$ we have the following possibilities:

1. $\Delta < 0$ (and then necessarily $e(x)d(x) < 0$). Then $h(x)$ is monotonic and the solutions of (3.1) are potentially oscillatory; when they are oscillatory, the $h(x)$ function is a tangent–like function, with zeros and singularities interlaced. In this case, one can enunciate both separation and comparison theorems.
2. $\Delta > 0$, then it is easy to check that the solutions may have one zero at most. We call this monotonic case. Sturm theorems are not available but we can derive bounds on the solutions using similar ideas.

3.2 Sturm Theorems

First we are considering the oscillatory case, in which $h(x)$ is a monotonic function with zeros and singularities interlaced. The following result holds:

Theorem 3.1 (Sturm separation theorem)**.** *Let $y(x)$ and $w(x)$ be nontrivial continuous solutions of the first order system with $d(x)$ and $e(x)$ continuous and not changing sign. Then, the zeros of y and w are simple and they are interlaced (between two zeros of each solution there is a zero of the other solution and only one).*

For a proof see [13]. An alternative way to see this result is noticing that if a solution has two zeros then necessarily $\Delta < 0$ and $d(x)e(x) < 0$ and then $h(x) = y(x)/w(x)$ is monotonic and continuous except at the zeros of $w(x)$. From this monotonicity, the interlacing of the zeros of $y(x)$ and $w(x)$ is obvious.

This simple result is interesting for studying interlacing properties of the zeros of special functions, as was investigated in [15]. By analyzing the continuity of the coefficients of the system we can deduce interlacing.

As an example, the following result was proved in [15].

Theorem 3.2. *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*

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

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 $p_{n-1}(x)$.

Many other results become available. To mention one example of interlacing between to different orthogonal sequences we have the following result for Jacobi polynomials.

Theorem 3.3. *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 $P_{\nu+1}^{(\alpha,-1)}(x)$.

Interlacing properties of the zeros of orthogonal polynomials have also been studied by K. A. Driver and collaborators using other techniques see [4–6]. Driver's et al. results include continuous shifts in the parameters (α and β for the case of Jacobi polynomials) but the profs are valid for orthogonal polynomials (ν integer) in the classical range of parameters ($\alpha, \beta > -1$ in the Jacobi case). In our case the parameters are shifted by integers but they apply to any solutions, not necessarily polynomials and not necessarily in the classical range. In this sense, the results are complementary.

Sturm comparison theorems can also be established by comparing the system with a system with constant coefficients. In order to simplify the discussion, we are considering a ystem of the form

$$\begin{aligned} y'(x) &= -\eta(x)y(x) + w(x) \\ w'(x) &= \eta(x)y(x) - y(x) \end{aligned} \tag{3.2}$$

with associated Riccati equation for $h(x) = y(x)/w(x)$

$$h'(x) = 1 - 2\eta(x)h(x) + h(x)^2. \tag{3.3}$$

We call this a system in reduced form; it has only one independent coefficient.

Considering systems in reduced form is not as restrictive as it may seems because it is always possible to transform a system with differential coefficients into a system in reduced form. [1]

We observe that the associated Riccati equation has solutions similar to a tangent function but with a parameter η which shrinks the function at one side of its zeros and expands it on the other side. Indeed, consider for instance (3.3) with $\eta > 0$, and a solution of this equation with a zero x_0. Let us compare this against $\tilde{h}(x) = \tan(x - x_0)$, solution of the auxiliary equation $\tilde{h}' = 1 + \tilde{h}^2$. We see that the slope of the solution of (3.3) is smaller than the slope of the solution of the auxiliary equation at the right of x_0 ($h > 0$), and that the contrary occurs at the left of x_0 ($h < 0$). This comparison with the tangent function immediately tells us that if x_y^i and $x_w^{(i)}$ denote zeros of y and w such that $x_w^{(1)} < x_y^{(1)} < x_w^{(2)}$ and $\eta > 0$ then

$$x_w^{(2)} - x_y^{(1)} > \frac{\pi}{2},\; x_y^{(1)} - x_w^{(1)} < \frac{\pi}{2}.$$

The contrary happens if $\eta < 0$. This result can be interpreted as a Sturm comparison theorem, and it was a crucial result in the construction of the numerical fixed point method of [13]. This type of result can be refined by comparing with equations with constant η but different from zero.

If η is monotonic, then it is possible to establish also Sturm convexity results, like for instance:

Theorem 3.4 (Sturm convexity)**.** *Let* $\{y(x), w(x)\}$ *as before and with* $|\eta(x)| < 1$, $\eta'(x) > 0$*. 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

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

The inequalities are reversed if $\eta'(x) < 0$*.*

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

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

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

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

with

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

4 First Order Differential Systems (Monotonic Case)

Now we turn our attention to monotonic systems (see Section 3.1). By the moment, let us consider the case $d(x)e(x) > 0$.

Because the solutions have one zero at most, we no longer have Sturm theorems; but a similar analysis used for proving Sturm theorems can be used to establish bounds on the solutions of monotonic systems.

As a first example, we consider the case of modified Bessel functions, described in detail in [17]. We have that both $y_\nu = e^{i\pi\nu} K_\nu(x)$ and $I_\nu(x)$ satisfy the system

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

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

with associated Riccati equation

$$h'_\nu(x) = 1 - \frac{2\nu-1}{x} h_\nu(x) - h_\nu(x)^2,\ h_\nu(x) = y_\nu(x)/y_{\nu-1}(x). \tag{4.1}$$

Now, solving $h'_\nu(x) = 0$ we see that

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

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

We concentrate on the $I_\nu(x)$ Bessel function, but similar ideas can be applied to $K_\nu(x)$. For the $I_\nu(x)$ function we see that 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 $d\lambda^+_\nu/dx > 0$ if $\nu \geq 1/2$, then, necessarily:

$$0 < \frac{I_\nu(x)}{I_{\nu-1}(x)} < \lambda^+_\nu(x),\ x > 0,\ \nu \geq 1/2. \tag{4.2}$$

Indeed, the initial conditions at $x = 0$ tells us that $0 < h_\nu(0^+) < \lambda^+(0^+)$, but this implies that $0 < h_\nu(x) < \lambda^+(x)$, $h_\nu(x) > 0$ for all $x > 0$. Indeed, the graph of $h_\nu(x)$ will never cut the graph of $\lambda^+(x)$ because $\lambda^+(x)$ is increasing. For this to happen at $x = x_t$ we would have that $h(x_t^-) < \lambda^+(x_t^-)$, $h(x_t) = \lambda^+(x_t)$ and $h'(x_t) = 0$; this is not possible because $\lambda^{+\prime}(x) > 0$. The situation is described in Figure 4.1 (dotted curve).

In [18], the more general case of monotonic systems

$$\begin{aligned} y'_n(x) &= a_n(x)y_n(x) + d_n(x)y_{n-1}(x) \\ y'_{n-1}(x) &= b_n(x)y_{n-1}(x) + e_n(x)y_n(x) \end{aligned} \tag{4.3}$$

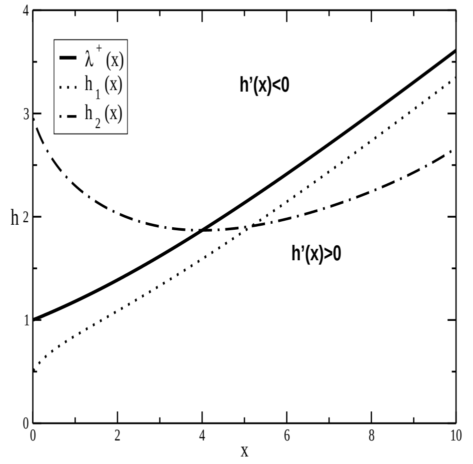

Figure 4.1: Two possible graphs for solutions of (4.1). The dotted curve is the situation for the ratio $h_\nu(x) = y_\nu(x)/y_{\nu-1}(x)$.

was considered. The case $e_n(x)d_n(x) > 0$ was considered, but also examples with $e_n(x)d_n(x) < 0$ were given.

The associated Riccati equation reads

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

In the analysis, it is important that the roots $\lambda^{\pm}(x)$ of the characteristic equation $h'(x) = 0$ are monotonic, but it was proved that this is true under conditions which are met quite generally. Indeed, it is easy to see that [18, Theorem 4] holds

Theorem 4.1. *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 $\lambda_n^{\pm}(x)$ *(the solutions of* $e_n(x)\lambda(x) + (b_n(x) - a_n(x))\lambda(x) - e_n(x)\lambda(x)^2 = 0$*) are monotonic in* (a, b). $d\lambda_n^{\pm}(x)/dx$ *have the same sign as* $A_{n-1}(x) - A_n(x)$ *and* $-\eta_n'(x)$.

Because of this, we were able to obtain, similarly as we did for modified Bessel functions, bounds for ratios of several important special functions, including modified

Bessel functions, parabolic cylinder functions and Hermite and Laguerre functions of negative argument. Similarly as for the case of the modified Bessel functions discussed before, these bounds are given by characteristic roots of the Riccati equation. From these bounds and using (4.3), also bounds for the logarithmic derivatives $y_n'(x)/y_n(x)$.

Is is also important to observe that in the usual scenario in which the shift $n \to n+1$ can be considered in (4.3), there is also a three-term recurrence relation associated to the system, namely:

$$e_{n+1}y_{n+1}(x) + (b_{n+1}(x) - a_n(x))y_n(x) - d_n y_{n-1}(x) = 0, \tag{4.4}$$

The characteristic roots for the recurrence are

$$e_{n+1}\bar{\lambda}_n^2 + (b_{n+1} - a_n)\bar{\lambda}_n - d_n = 0, \tag{4.5}$$

and it is a classical result that the asymptotic behavior an $n \to +\infty$ is precisely determined by these characteristic roots. This is certified by the Perron–Kreuser theorem (see, for instance, [8, Theorem 4.5]).

Theorem 4.2 (Perron–Kreuser)**.** *If* $\lim_{n\to+\infty} |\bar{\lambda}_n^{(+)}/\bar{\lambda}_n^{(-)}| \neq 1$ *with* $\bar{\lambda}_n^{(\pm)}$ *the solutions of* $\alpha_n\lambda_n^2 + \beta^2\lambda_n + \gamma_n = 0$*, then solutions* $\{y_k^{(1)}, y_k^{(2)}\}$ *of the recurrence* $\alpha_n y_{n+1} + beta_n y_n + \gamma_n y_{n-1} = 0$ *exist such that*

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

An important observation is that the characteristic roots of the recurrence relation (4.4) are very similar to the roots for the Riccati equation (solutions of (4.5)), which are function bounds (like, for example, in (4.2)). This means that these bounds tend to be more accurate as $n \to +\infty$ and that in the limit they reproduce the correct asymptotic behavior. On the other hand, these bounds are also related to the Liouville–Green transformation [20], and they are usually also more accurate as x becomes large.

Another important consequence of the existence of a recurrence relation is that it can be used to generate sequences of bounds, which are 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. Similarly, the forward iteration gives sequences of bounds for dominant solutions (nonconvergening sequences).

And because upper and lower bounds, it is also possible to establish Turán-type inequalities in the following way:

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

In [18], we can find a good number of applications of these ideas. We mention a few applications for the case $d(x)e(x) > 0$.

1. A Turán-type inequality for modified Bessel functions $K_\nu(x)$:

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

   This result was proved independently, and using different techniques, in [1, 17].

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

   Theorem 4.3. *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 $n = -1/2$.

   Theorem 4.4 (Turán-type inequalities for PCFs)**.** *Let*

$$F(x) = \frac{U(n,x)^2}{U(n-1,x)U(n+1,x)}.$$

   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 $n \in (-1/2, 1/2)$.

   Theorem 4.5 (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 is

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

   where

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

3. Some Turán-type inequalities for orthogonal polynomials outside the interval of orthogonality

   (a) Hermite polynomials

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

   (b) Associated Legendre functions of imaginary variable

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

   (c) Laguerre functions

   Theorem 4.6. *For any $\nu \geq 0$ and $\alpha \geq 0$, $x > 0$ the following holds:*

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

We also gave some examples of application for monotonic cases with $e(x)d(x) < 0$ and described how the bounds could be used to establish bounds on the extreme zeros of orthogonal polynomials. The cases described by no means exhaust the examples to which these ideas can be applied. And to illustrate this, we consider a brief example of application to incomplete gamma functions.

4.1 Bounds for the Incomplete gamma Function $\gamma(\alpha, x)$

The incomplete gamma function $\gamma(a, x)$, which is defined as

$$\gamma(a,x) = \int_0^x t^{a-1}e^{-t}dt, \tag{4.6}$$

satisfies the recurrence relation (Paris [8.8.3])

$$\gamma(a+2,x) - (a+1+x)\gamma(a+1,x) + ax\gamma(a,x) = 0 \tag{4.7}$$

and the differential relation [Paris, 8.8.15]

$$\frac{d^n}{dx^n}(x^{-a}\gamma(a,x)) = (-1)^n x^{-n-a}\gamma(a+n,x). \tag{4.8}$$

With this we arrive to the system

$$\begin{aligned} \frac{d}{dz}\gamma(a,x) &= -\gamma(a,x) + (a-1)\gamma(a-1,x) \\ \frac{d}{dz}\gamma(a-1,x) &= \frac{a-1}{x}\gamma(a-1,x) - \frac{1}{z}\gamma(a,x). \end{aligned} \tag{4.9}$$

From this, the ratio

$$h_a(x) = \gamma(a,x)/\gamma(a-1,x) \tag{4.10}$$

satisfies:

$$h'_a(x) = (a-1) - \left(1 + \frac{a-1}{x}\right) h_a(x) + \frac{1}{x} h_a^2(x). \tag{4.11}$$

We see that the characteristic roots are $\lambda_1(x) = x$ and $\lambda_2(x) = a-1$. But because for the ratio (4.10) we have, using [Paris, 8.7.1],that $h_a(0^+) = 0^+$ and $h'_a(0^+) > 0$ if $a > 1$ ($h_a(z) = (a-1)z/a + \mathcal{O}(z^2)$ of $a > 1$), graphical arguments easily gives us that

Theorem 4.7. *For $a > 1$ and $x > 0$ the following holds:*

$$h_a(x) = \frac{\gamma(a,x)}{\gamma(a-1,x)} < \min\{a-1, x\} \leq x, \tag{4.12}$$

$$h'_a(x) > 0. \tag{4.13}$$

This result finds a similar explanation to other similar results, like Eq. (4.2). For $x > 0$ $\gamma(a,x) > 0$, and from (4.11) we observe that the positive solutions of the Riccati equation are such that $h'_a(x) > 0$ only if $h_a(x) < x$ when $x \leq a-1$ and $h_a(x) < a-1$ when $x > a-1$. Then, because for $h_a(x)$ in (4.10) we have that $h'_a(0^+) > 0$ and the graph of $h_a(x)$ can not intersect with the graph of the characteristic roots from below (because they are nondecreasing functions) then, necessarily, $h'_a(x) > 0$ for $x > 0$ and consequently $h_a(x) < x$ if $x < a-1$ and $h_a(x) < a-1$ for $x \geq a-1$.

Now we prove the following result

Theorem 4.8. *The ratio $h_a(x) = \gamma(a,x)/\gamma(a-1,x)$ is increasing as a function of a if $a > 1$, $z > 0$.*

Proof. We assume $a > 1$. We start by noticing that $h_{a+\epsilon}(0^+) = h_a(0^+) = 0^+$, $\epsilon > 0$, but that $h'_a(0^+) = 1 - 1/a < h'_{a+\epsilon}(0^+)$. Therefore we will have $h_{a+\epsilon}(x) > h_a(x)$ for x sufficiently close to $x = 0$; but then it is easy to see that this must hold for any $x > 0$. Too see this, let us assume $h_{a+\epsilon}(x_e) = h_a(x_e)$ and $h_{a+\epsilon}(x) > h_a(x)$ for $x \in (0, x_e)$ and we will arrive at a contradiction. Indeed, this immediately implies that $h'_{a+\epsilon}(x_e) < h'_a(x_e)$ and with $h_{a+\epsilon}(x_e) = h_a(x_e)$ but this is in contradiction with the equation (4.11), because for a same value of h_a (fixed) the derivative h'_a increases with a. This can be checked by taking the partial derivative of h_a with respect to a with z and h_a fixed:

$$\frac{\partial h'_a(x)}{\partial a} = 1 - h_a(z)/z > 0$$

where we have used theorem (4.7) in the inequality. □

Taking into account the previous theorem, we arrive to the following corollary

Corollary 4.9. *$\gamma(a,x)/\gamma(a-1,x)$, $a > 1$, $x > 0$ is increasing both as a function of x and a.*

This result is not new [12], but here we have proved it in a very elementary way.

5 Numerical Applications: Computing Zeros of Special Functions

Finally, we describe in this last section the application of Sturm theorems for the computation of the zeros of special functions. It is very surprising that, in spite of the many applications to the analysis of the zeros of special functions, Sturm theorems had not been considered as numerical tools for their computation until very recently. The resulting methods are simple to implement and they are very fast and totally reliable.

5.1 Methods for First Order Systems

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 [13]; the foundation of these methods are the Sturm separation theorem and the Sturm comparison theorems described in Section 3.2.

We are not describing in detail these methods and we move to the recent and more powerful fourth order methods based on Sturm theorems for second order ODEs.

5.2 A Fourth Order Method for the Real Zeros of Solutions of Second Order ODEs

Theorem 2.4 is the main tool for constructing a method to compute with certainty all real zeros of any solution of an ODE

$$y''(x) + A(x)y(x) = 0 \tag{5.1}$$

in any interval where $A(x)$ is continuous and monotonic. The restriction to normal form (no first derivative) is soft, because we can transform to normal form using Liouville transformations (see Section 2.1). About the monotonicity, we can also divide an interval in different subintervals were $A(x)$ is monotonic and apply the method in each of these subintervals; in any case, we will require that the monotonicity properties of $A(x)$ can be obtained.

As an immediate consequence of Theorem 2.4, we obtain a method to compute with certainty all the zeros in an interval were $A(x)$ is monotonic.

Algorithm 5.1 (Zeros of $y''(x) + A(x)y(x) = 0$, $A(x) > 0$ monotonic). Starting from a given x_0, we compute successive iterates as follows. Given x_n, 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. If α is the zero of $y(x)$ closest to x_0 and large (smaller) than x_0, the sequence $\{x_n\}$ converges to α.

This algorithm generates a monotonic sequence, increasing if $A'(x) < 0$ and decreasing if $A'(x) > 0$, converging with certainty to a zero. The reason why this is so is easy to understand from the Sturm theorem. Indeed, if, for instance, $A'(x) < 0$, then the zero of the solution of $w''(x) + A(x_n)w(x) = 0$ larger than x_n and closer to x_n is smaller than the zero of α because $A(x) < A(x_n)$ if $x > x_n$. Then $x_n < x_{n+1} < \alpha$.

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

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

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 $A'(x) > 0$).

After a zero α has been computed, Sturm theorem gives us a valid guess for computing the next zero. If, for instance $A'(x) < 0$, and β is the next zero larger than α, then

$$x_0 = \alpha - j\pi/\sqrt{A(\alpha)},\ j = \text{sign}\left(A'(x)\right) \tag{5.2}$$

is such that $x_0 \in (\alpha, \beta)$ because $A(x) < A(\alpha)$ if $x > \alpha$ (see Theorem 2.3). Starting form this x_0 and applying again Algorithm 5.1, we obtain convergence to β. In this way we can compute all the successive zeros in an interval where $A(x)$ is monotonic.

For $A'(x) > 0$ the same ideas can be applied but the zeros are computed in decreasing order. Combining the fixed point iteration with the step (5.2) we obtain the following algorithm:

Algorithm 5.2. Computing zeros for $A(x)$ monotonic in an interval $[a, b]$. Repeat until a value of x outside the interval $[a, b]$ is reached:

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.

A simple example of computation with this algorithm is shown in Fig. 5.1 for an elementary case: the zeros of $y(x) = x\sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$.

The method does not only converge with certainty, but it does also converge in a fast way. The method has fourth order convergence; indeed, it is easy to check that

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

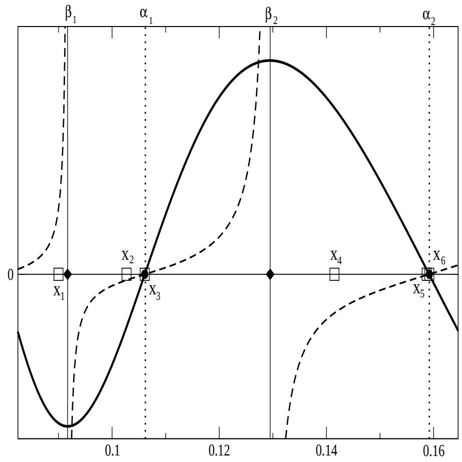

Figure 5.1: Computation of the zeros of $y(x) = x\sin(1/x)$, solution of $y''(x) + x^{-4}y(x) = 0$, with four digits accuracy. The sequence of operations is $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ ($x[3]$ provides four digits) $x[4] = x[3] + \pi/A(x[3])$ (smaller than the next zero by Sturm comparison) $T(x[4]) = x[5]$, $T(x[5]) = x[6]$ ($x[6]$ provides four digits)

Apart from this, the method was proved to have good nonlocal convergence in the sense that, once a zero is computed, the estimation for the next zero (5.2) produces convergence in few iterations. The method has fast convergence due to its fourth order and good nonlocal behavior, requiring typically only 3 or 4 iterations for computing with 100-digits accuracy. Additionally, the algorithm computes with certainty all the zeros in each subinterval where $A(x)$ is monotonic.

The main requirement is that the monotonicity properties of the coefficient $A(x)$ are known in advance. Fortunately, and as explained in Section 2.1, this work has already been carried out for Gauss and confluent hypergeometric functions and considering different changes of variable [2, 3]; in that cases, these properties can be analyzed just by to solving of a second order algebraic equation.

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

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

For computing these zeros, we first obtain the second order ODE satisfied by $\tilde{y}(x) = y'(x)$, $y(x) = x^\gamma\mathcal{C}_\nu(x)$, transform to normal form with a change of function and then solve the monotonicity. After this, the fourth order method can be applied. In this case studying of the monotonicity of the resulting coefficient $A(x)$ implies solving cubic equations [11]. The resulting method is very efficient and it is reliable, also for the computation of double zeros [7].

5.3 Computing Complex Zeros of Special Functions

It is possible to extend the previous fourth order method to zeros in the complex plane. We start considering the trivial case of $A(z)$ constant. Then the general solution of $w''(z)+A(z)w(z)=0$ reads

$$w(z)=C\sin\left(\sqrt{A(z)}(z-\psi)\right),$$

and the zeros are over the line

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

In other words, the zeros are over an integral line of

$$\frac{dy}{dx}=-\tan(\varphi/2). \tag{5.3}$$

The method for complex zeros is based on the assumption that if $A(z)$ is not constant the curves where the zeros lie will be approximately given by (5.3), but with variable φ. This assumption is equivalent to consider that the Liouville–Green (or WKB) approximation is accurate. The WKB approximation with a zero at $z^{(0)}$ is

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

and other zeros lie over the curve such that

$$\Im\int_{z^{(0)}}^{z}A(\zeta)^{1/2}d\zeta=0. \tag{5.4}$$

Those curves are also given by (5.3). These are the so-called anti-Stokes lines (ASLs).

The method for computing complex zeros follows the path of the ASLs and it is similar to the method for real zeros. Given $z^{(0)}$ ($y(z^{(0)})=0$) and assuming that $|A(z)|$ decreases for increasing $\Re z$ we consider the following algorithm to compute the next zero:

Algorithm 5.3. Basic algorithm for complex zeros; $|A(z)|$ decreasing.

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

$$T(z)=z-\frac{1}{\sqrt{A(z)}}\arctan\left(\sqrt{A(z)}\frac{w(z)}{w'(z)}\right). \tag{5.5}$$

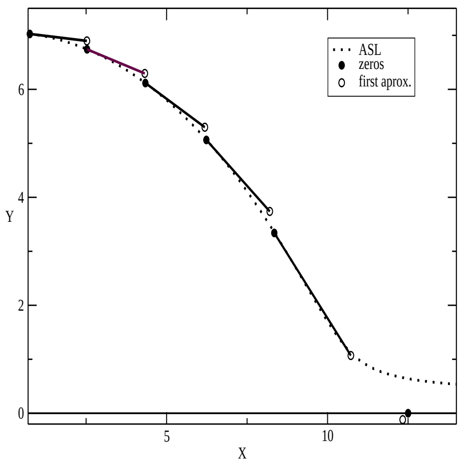

Figure 5.2: Zeros of the Bessel function $Y_{10.35}(z)$ in the quadrant $\Re z > 0$, $\Im z > 0$ (black circles), and first estimations to the zeros (white circles); the dotted line is the anti–Stokes line passing through the zero with larger imaginary part.

3. Take as approximate zero $\alpha = z_{n+1}$ and $z_0 = \alpha$. Go to 1.

We observe that if $A(z)$ has slow variation, the first step might be a good approximation to $z^{(1)}$. In addition, the step is tangent to the anti-Stokes line (ASL) at $z^{(0)}$ (that is: the straight line joining $z^{(0)}$ and z_0 is tangent at $z^{(0)}$ to the ASL passing through this point). That the first step is a good approximation to $z^{(1)}$ will depend on how accurate is the WKB approximation. On the other hand, $T(z)$ is a fixed point iteration with order of convergence 4, and this fact does not depend on the validity of the WKB approximation.

Figure 5.2 shows the complex zeros of the Bessel function $Y_{10.35}(z)$ in the first quadrant, the first estimations provided by the method together with the ASL passing through the zero with largest imaginary part. The algorithm starts with this zero and computes the following zeros (with successively smaller imaginary parts). The zeros are very close to the ASL and the first estimations are very reasonable, except that after computing the last zero with positive imaginary part the estimation for the next zero (which is on the real line) is not accurate. Furthermore, this zero appears well separated from the ASL. We conclude that the WKB approximation works initially well but that it is not accurate for computing the last zero (although the iteration finally converges to this zero). The problem with this last zero is that WKB fails as a principal Stokes line is crossed.

The way to avoid computing zeros which are separated from the initial anti-Stokes line is to divide the problem in different sectors in the complex plane in such a way that a principal Stokes lines are not crossed. For more details and some explicit algorithms, we refer to [19].

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