RELIABLE COMPUTATION OF THE ZEROS OF SOLUTIONS OF SECOND ORDER LINEAR ODEs USING A FOURTH ORDER METHOD*

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Abstract. A fourth order fixed point method to compute the zeros of solutions of second order homogeneous linear ODEs is obtained from the approximate integration of the Riccati equation associated with the ODE. The method requires the evaluation of the logarithmic derivative of the function and also uses the coefficients of the ODE. An algorithm to compute with certainty all the zeros in an interval is given which provides a fast, reliable, and accurate method of computation. The method is illustrated by the computation of the zeros of Gauss hypergeometric functions (including Jacobi polynomials) and confluent hypergeometric functions (Laguerre polynomials, Hermite polynomials, and Bessel functions included) among others. The examples show that typically 4 or 5 iterations per root are enough to provide more than 100 digits of accuracy, without requiring a priori estimations of the roots.

1. Introduction. Many methods with different characteristics are available to solve nonlinear equations $f(x) = 0$, from the safe and generally slow bisection method to many fast, but more unpredictable, higher order methods such as the Newton–Raphson method.

In order to compute all the zeros of a real function $f(x)$ in a real interval, it is generally necessary that the zeros become isolated inside bracketing intervals (enough for bisection) or that sufficiently accurate first approximations to the roots are available as starting values. The second possibility is usually considered before applying Newton–Raphson or other higher order methods. For instance, this is the approach used to compute zeros of some orthogonal polynomials [24] and Bessel functions [21]. However, it is generally difficult to find sufficiently accurate approximations for all the zeros, particularly when the function $f(x)$ may depend on several parameters; and it is very difficult to be sure that convergence is always certain for any parameter values and for any zero. See [19] for the one parameter case of Legendre polynomials.

Another possibility is more specialized methods requiring less specific information on the location of the zeros. Methods are available for certain types of functions which require neither bracketing nor a priori approximations.

A first important class of functions is that of the solutions of linear homogeneous second order difference equations, and specific methods exist for some of these solutions. In particular, for the important case of orthogonal polynomials $p_k(x)$ (k is the degree), the zeros can be obtained as eigenvalues of real tridiagonal symmetric matrices [11] with entries easily obtained from the coefficients of the three-term recurrence relation $p_{n+1}(x) = (A_n x + B_n)p_n(x) + C_n p_{n-1}(x)$. For some nonpolynomial

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functions, it is also possible to obtain the zeros as approximate eigenvalues of real tridiagonal symmetric matrices; this is the case for some minimal solutions of three-term recurrence relations. Examples are the regular Bessel [12] and Coulomb wave functions [14].

A second class is that of the functions satisfying first order linear homogeneous difference-differential equations (DDEs). Fixed point methods (FPMs) can be obtained from the approximate integration of Riccati equations associated with the DDEs [20, 8]. The methods are globally convergent, have order two, and can be used to compute with certainty all the real zeros in an interval. The methods apply to all the cases for which the matrix eigenvalue methods are successful but are not limited to them. Combining these DDE methods with an FPM to locate the extrema (based on the associated ODE), second order methods can be obtained to compute the zeros of the solutions of the DDEs and those of the first derivative (see [8]).

We refer the reader to [10, Chap. 7] for a detailed analysis of the DDE methods and the matrix eigenvalue methods.

A third set of functions, and probably the most important one, is that of the functions which are solutions of linear second order homogeneous ODEs. This set includes all the functions for which the matrix eigenvalue and the DDE methods have been applied, but it is not limited to them. In this paper, we present a fourth order method that is globally convergent under certain monotonicity conditions. This is a remarkable property for a fourth order method. The method is based on the approximate integration of a Riccati equation associated with the ODE and requires, as does Newton's method, the evaluation of the logarithmic derivative of the problem function. The coefficients of the ODE are also used in the computation.

Based on this iterative method, we will construct an algorithm to compute with certainty all the zeros in any real interval. Initial estimations for each zero are not needed because of the global convergence. The only requirement is that information on the monotonicity of the coefficients of the ODE is available. In particular, for second order ODEs in normal form, $y''(x) + A(x)y(x) = 0$, it is required that the sign of $A'(x)$ and its possible changes are known in advance.

This provides an efficient method to compute the real zeros of a large number of important functions. As we will see, the method is able to compute the zeros with 100-digit accuracy typically with only 4–5 iterations per root, clearly outperforming the already fast global methods based on DDEs [20, 8]. Of course, when accurate estimations for the zeros are known, they can be used in conjunction with the method. However, the new method is fast and simple and does not require specific starting values for each zero; it gives a general scheme valid for any solution of the ODE.

The structure of the paper is as follows. In section 2 a fixed point method of order four is obtained that shows some monotonic convergence properties when $A(x)$ is monotonic; the method is globally convergent under certain restrictions on the speed of variation of $A(x)$. In section 3, the fixed point method is modified, and a globally convergent iteration is obtained. Using this modified iteration, an algorithm to compute with certainty all the zeros in an interval is developed; also, how to compute the zeros of the derivative is discussed. In section 4, the nonlocal behavior of the algorithm is studied, and the particular (but important) case $y''(x) + x^{-m}y(x) = 0$, $m \in \mathbb{R}$, is analyzed in detail. In section 5, the performance of the algorithm is illustrated by examples, including the classical orthogonal polynomials (Hermite, Laguerre, and Jacobi), Coulomb wave functions, Bessel functions of real or imaginary orders and variables, and conical functions.

2. Approximate integration of the second order ODE and FPM. We consider a generic equation in normal form:

$$(2.1) \qquad\qquad y''(x) + A(x)y(x) = 0.$$

For the case of an equation in standard form,

$$(2.2) \qquad\qquad v''(x) + \tilde{B}(x)v'(x) + \tilde{A}(x)v(x) = 0,$$

it is well known that the function

$$(2.3) \qquad\qquad y(x) = \exp\left(\frac{1}{2}\int \tilde{B}(x)dx\right)v(x)$$

satisfies an equation in normal form (2.1) with

$$(2.4) \qquad\qquad A(x) = \tilde{A}(x) - \frac{\tilde{B}(x)^2}{4} - \frac{\tilde{B}'(x)}{2}.$$

Next, we will obtain a method to compute the zeros of solutions of (2.1) in intervals where $A(x) > 0$, where more than one zero may occur. The method computes all the zeros in these intervals without missing any. The zeros in intervals where $A(x) < 0$ are isolated zeros (only one zero in the interval); in section 3.1 we give more details on the computation of these isolated zeros.

Considering that $A(x) > 0$, we find that the function $h(x) = y(x)/y'(x)$ satisfies the Riccati equation

$$(2.5) \qquad\qquad h'(x) = 1 + (w(x)h(x))^2,$$

where $w(x) = \sqrt{A(x)}$.

Because $A(x) > 0$, the zeros of $y(x)$ and $y'(x)$ are simple, and they are interlaced (between two zeros of $y(x)$ there is one and only one zero of $y'(x)$, and vice versa); therefore, the graph of $h(x)$ has a shape similar to that of a tangent function, with zeros and singularities interlaced.

Let α be such that $y(\alpha) = 0$. We can integrate (2.5) around α by setting

$$(2.6) \qquad\qquad \int_{\alpha}^{x} \frac{h'(\zeta)}{1 + (w(\zeta)h(\zeta)^2)}d\zeta = x - \alpha,$$

where x is such that $h(x)$ is continuous between α and x. Now, let us consider the approximation in which $w(x) = W$ is constant and compute the integral. We have, because $h(\alpha) = 0$,

$$(2.7) \qquad\qquad \frac{1}{W}\arctan(Wh(x)) \approx x - \alpha,$$

where, as usual, $\arctan(z) \in (-\pi/2, \pi/2)$.

Now, setting again $W = w(x)$, we have

$$(2.8) \qquad\qquad \alpha \approx x - \frac{1}{w(x)}\arctan(w(x)h(x)).$$

This approximation of α can be improved by iteration. Thus, we consider the FPM

$$x_{n+1} = g(x_n), \quad g(x) = x - \frac{1}{w(x)}\arctan(w(x)h(x)),$$

$$(2.9)$$

$$w(x) = \sqrt{A(x)}, \quad h(x) = y(x)/y'(x).$$

This FPM is locally convergent because $|g'(x)| < 1$ around α (which is enough to ensure local convergence; see, for instance, [10, sect. 7.2.2]). Indeed, taking the derivative and using (2.5), we find

(2.10)
$$g'(x) = f(x)K(\phi(x)), \quad \phi(x) = w(x)h(x),$$

$$f(x) = \frac{w'(x)}{w(x)^2}, \quad K(z) = \arctan(z) - \frac{z}{1 + z^2}.$$

Then, because $K(0) = 0$, $g'(\alpha) = 0$, and convergence is guaranteed, at least locally. Next, we prove that the method is of fourth order.

2.1. Order of the method. In order to obtain the order of the method, we have to compute the derivatives of $g(x)$ (see (2.9)) at $x = \alpha$.

Let us recall that if the first nonvanishing derivative for an FPM $x_{n+1} = g(x_n)$ is $g^{(m)}(\alpha)$, by expanding in Taylor series the error $\epsilon_{n+1} = x_{n+1} - \alpha$, it is found that the method has order m with asymptotic error constant $g^{(m)}(\alpha)/m!$. Indeed, we have

(2.11) $$\epsilon_{n+1} = x_{n+1} - \alpha = g(\alpha + \epsilon_n) - g(\alpha) = \frac{g^{(m)}(\alpha)}{m!}\epsilon_n^m + \mathcal{O}(\epsilon_n^{m+1}).$$

In the case of the FPM (2.9), it is straightforward to show that

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

and therefore

(2.13) $$\epsilon_{n+1} = \frac{A'(\alpha)}{12}\epsilon_n^4 + \mathcal{O}(\epsilon_n^5).$$

The derivatives (2.12) follow from (2.10), assuming that $w(x)$ is sufficiently differentiable around α and taking into account that $h(\alpha) = 0$. With this and considering that

(2.14) $$K(0) = \frac{dK}{dz}(0) = \frac{d^2K}{dz^2}(0) = 0, \quad \frac{d^3K}{dz^3}(0) = 4,$$

using the chain rule it becomes obvious that $g'(\alpha) = g''(\alpha) = g'''(\alpha) = 0$ and that the only term that survives in the fourth derivative is

(2.15) $$g^{(4)}(\alpha) = f(\alpha)[\phi'(\alpha)]^3\frac{d^3K}{dz^3}(0) = 4w(\alpha)w'(\alpha).$$

Therefore, (2.12) holds and the method is of order 4 with asymptotic error constant $A'(\alpha)/12$. This means that, roughly speaking, the number of correct digits is increased by a factor of 4 in each iteration (as long as the iterates are close enough to α).

2.2. Monotonic and global convergence properties. Next we show that the FPM (2.9) has "half-global" monotonic convergence properties if the coefficient $A(x)$ is monotonic and that, under mild conditions on the speed of variation of $A(x)$, the method becomes globally convergent. Furthermore, with a simple modification of (2.9) the method becomes globally and monotonically convergent, without limitations on the speed of variation of $A(x)$. This is the basis of the algorithm to compute all the zeros in any real interval (section 3).

The following result [8, Corollary 3.3] will be useful.

LEMMA 2.1. *Let $y(x)$ be a solution of $y''(x) + A(x)y(x) = 0$. Let α and β be zeros of $y(x)$ and $y'(x)$, respectively, such that $y(x) \neq 0$ and $y'(x) \neq 0$ between α and β. If $0 < k < A(x) < K$ between α and β, then*

$$\frac{\pi}{2\sqrt{K}} < |\alpha - \beta| < \frac{\pi}{2\sqrt{k}}.$$

In the next theorem, the first two results are what we call the "half-global" monotonic convergence properties, and the third result is the global convergence property.

THEOREM 2.2. *Let $y(x)$ be a solution of $y''(x) + A(x)y(x) = 0$, and let β_1 and β_2 be two zeros of $y'(x)$ such that $A(x) > 0$ in $[\beta_1, \beta_2]$. Let α be the only zero of $y(x)$ in (β_1, β_2).*

Then the following hold:
1. *If $A'(x) > 0$ in (α, β_2), where $h(x) > 0$, then the sequence (2.9) converges monotonically to α for any $x_0 \in (\alpha, \beta_2)$.*
2. *If $A'(x) < 0$ in (β_1, α), where $h(x) < 0$, then the sequence (2.9) converges monotonically to α for any $x_0 \in (\beta_1, \alpha)$.*
3. *If $A(x)$ is monotonic and $1/4 < A(\beta_1)/A(\beta_2) < 4$, then the sequence (2.9) converges to α for any $x_0 \in (\beta_1, \beta_2)$.*

Proof. We consider the case $A'(x) < 0$, and we prove the second and the third results; the discussion for $A'(x) > 0$ is similar.

From (2.10) and because $w'(x) < 0$ and $\text{sign}(K(z)) = \text{sign}(z)$, we have that $\text{sign}(g'(x)) = -\text{sign}(h(x))$. Therefore, $g'(x) > 0$ in (β_1, α) because $h(x) < 0$ in this interval; this implies monotonic convergence for starting values $x_0 \in (\beta_1, \alpha)$. Indeed, using the mean value theorem, we have

$$(2.16) \qquad \alpha - x_1 = g(\alpha) - g(x_0) = g'(\zeta)(\alpha - x_0) > 0,$$

where ζ is some value in the interval (x_0, α). Therefore, $x_1 < \alpha$ and also, considering (2.9), $x_0 < x_1 = g(x_0)$. Then, by induction we see that $x_0 < \cdots < x_n < \alpha$ for any $n \in \mathbb{N}$, and $\{x_n\}$ is a monotonically increasing sequence with an upper bound and thus converges monotonically (necessarily to the fixed point α). This proves the first statement of the theorem.

On the other hand, if $x_0 \in (\alpha, \beta_2)$, because $g'(\zeta) < 0$ for $\zeta \in (\alpha, \beta_2)$, then we have

$$(2.17) \qquad \alpha - x_1 = g'(\zeta)(\alpha - x_0) > 0$$

and $x_1 < \alpha$; therefore, monotonic convergence does not occur because $x_0 > \alpha$ and $x_1 < \alpha$. But if, in addition, $x_1 > \beta_1$, then monotonic convergence occurs after the first iteration on account of the second result of the theorem. Now we find a sufficient condition for this to happen (the third result of the theorem).

Because $g'(x) < 0$ in (α, β_2), the smallest possible value of x_1 when $x_0 \in (\alpha, \beta_2)$ corresponds to the largest possible x_0 in this interval, that is, for $x_0 \to \beta_2^-$. Then, if $g(\beta_2^-) > \beta_1$, we will have monotonic convergence to α after the first iteration. This happens when

$$(2.18) \qquad \beta_2 - \frac{\pi}{2\sqrt{A(\beta_2)}} > \beta_1.$$

Using Lemma 2.1 and because $A(x)$ is decreasing, $\beta_2 - \beta_1 = \beta_2 - \alpha + \alpha - \beta_1 > \pi/(2\sqrt{A(\alpha)}) + \pi/(2\sqrt{A(\beta_1)})$. Therefore, (2.18) is satisfied, and convergence is guaranteed whenever $A(\beta_2)^{-1/2} < A(\alpha)^{-1/2} + A(\beta_1)^{-1/2}$, and because $A(\alpha) < A(\beta_1)$ this inequality is certainly satisfied if $A(\beta_2)^{-1/2} < 2A(\beta_1)^{-1/2}$, and the result is proved. $\square$

3. Computing all the zeros in an interval with globally convergent iterations. From Theorem 2.2, we learn that when $A(x) > 0$ and $A'(x) < 0$, convergence is certain and monotonic for starting values on the left of the zero α ($x_0 \in (\beta_1, \alpha)$), but that for starting values on the right we need that $A(x)$ varies mildly; the opposite occurs when $A'(x) > 0$. We can extend these lateral convergence properties by a convenient redefinition of the range of the arctan function. Given an interval where $A(x)$ is positive and monotonic, the new method will be convergent to a zero (if it exists) in the interval for any starting value in this interval and without restrictions on the speed of variation of $A(x)$.

We consider

$$(3.1) \qquad \arctan_j(\zeta) = \begin{cases} \arctan(\zeta), & j\zeta > 0, \\ \arctan(\zeta) + j\pi, & j\zeta \leq 0, \end{cases} \quad j = \pm 1,$$

and define new iterations as follows:

$$(3.2) \quad x_{n+1} = T_j(x_n), \, T_j(x) = \begin{cases} x - \dfrac{1}{w(x)} \arctan_j(w(x)h(x)) & \text{if } y'(x) \neq 0, \\ x - \dfrac{1}{w(x)} j\dfrac{\pi}{2} & \text{if } y'(x) = 0, \end{cases}$$
$$j = \text{sign}(A'(x)).$$

In other words, we modify (2.9) by considering that the range of arctan is $(0, \pi/2) \cup (\pi/2, \pi]$ when $A'(x) > 0$ ($j = +1$) and $[-\pi, -\pi/2) \cup (-\pi/2, 0)$ when $A'(x) < 0$ ($j = -1$), and we define $T_j(x)$ at the zeros of $y'(x)$ in such a way that $T_j(x)$ is continuous and differentiable around these zeros.

Then, we have the following global convergence properties.

THEOREM 3.1. *Let $y(x)$ be a solution of $y''(x) + A(x)y(x) = 0$ with two consecutive zeros α_1 and α_2 such that $A(x) > 0$ in $[\alpha_1, \alpha_2]$. Then the following hold:*
  1. *If $A'(x) > 0$ in (α_1, α_2), then the sequence (3.2) converges monotonically to α_1 for any $x_0 \in (\alpha_1, \alpha_2]$.*
  2. *If $A'(x) < 0$ in (α_1, α_2), then the sequence (3.2) converges monotonically to α_2 for any $x_0 \in [\alpha_1, \alpha_2)$.*

The order of convergence is 4.

Proof. We consider the case $A'(x) < 0$ (and therefore $j = -1$ in (3.2)).

We define $\bar{T}_{-1}(x) = T_{-1}(x)$ for $x \in [\alpha_1, \alpha_2)$ and $\bar{T}_{-1}(\alpha_2) = \alpha_2$ (notice that $T_{-1}(\alpha_2) \neq \alpha_2$). Then, $\bar{T}_{-1}(x)$ is continuous in $[\alpha_1, \alpha_2]$ and differentiable in (α_1, α_2), where $\bar{T}'_{-1}(x) > 0$ (the derivative $\tilde{T}'_{-1}(x)$ is the same as $g'(x)$ (2.10) but with arctan replaced by (3.1)).

Now, let $x_0 \in [\alpha_1, \alpha_2)$. We have $x_1 = T_{-1}(x_0) = \bar{T}_{-1}(x_0) > x_0$. In addition,

$$(3.3) \qquad \alpha_2 - x_1 = \bar{T}_{-1}(\alpha_2) - \bar{T}_{-1}(x_0) = \bar{T}'_{-1}(\zeta)(\alpha_2 - x_0) > 0$$

(ζ a value in (x_0, α_2)). Therefore, $x_0 < x_1 < \alpha_2$, and, repeating the argument, $x_0 < \cdots < x_n < \alpha$ for all n, which proves that the sequence defined by $x_{n+1} = T_{-1}(x_n) = \bar{T}_{-1}(x_n)$ converges monotonically to α_2 (fixed point of $\bar{T}_{-1}(x)$).

The order of convergence is four, as it was for (2.9), because $T_{-1}(x) = g(x)$ in (β, α_2), β being the only zero of $y'(x)$ between α_1 and α_2. □

Remark 1. In the previous theorem, when $A'(x) < 0$ the result is also true for any interval $[a, \alpha_2)$ with a such that $y(x) \neq 0$ in (a, α_2). If $A'(x) > 0$, the theorem also holds in intervals $(\alpha_1, b]$ where $y(x) \neq 0$.

Observe that, in contrast to (2.9), the zeros of $y(x)$ are not fixed points of $T_j(x)$. If α is a zero of $y(x)$, then $T_j(\alpha) = \alpha - j\pi/\sqrt{A(\alpha)}$.

Using $T_j(x)$, it is easy to write an algorithm to compute all the zeros in an interval $[a, b]$ where $A(x)$ is positive and monotonic. For instance, if $A'(x) < 0$, then we start with $x_0 = a < \alpha_1$ and iterate until convergence to a zero α_1 is obtained. Then, with $x_0 = \alpha_1$ we iterate again (the first iteration being $x_1 = T_{-1}(\alpha_1) = \alpha_1 + \pi/\sqrt{A(\alpha_1)}$), and we will have convergence to the next zero $\alpha_2 > \alpha_1$, and so on.

Because the zeros α_i will not be computed exactly, in the algorithm it is convenient to use an alternative notation for $T_j(\alpha_i)$. We will use $S_{j\pi}(\alpha_i)$, where

$$(3.4) \qquad\qquad S_{j\pi}(x) = x - j\frac{\pi}{\sqrt{A(x)}}$$

(of course, $S_{j\pi}(\alpha_i) = T_j(\alpha_i)$).

ALGORITHM 1 (decreasing and positive $A(x)$).
Input: interval $[a, b]$, relative error tolerance ϵ
Output: zeros $\alpha[i]$ in increasing order ($\alpha[1] < \alpha[2] < \cdots$)
1. *$x = a$; $i = 0$;*
2. *While $x < b$*
3.   *$\Delta = \epsilon + 1$;*
4.   *While ($\Delta > \epsilon$ and $x < b$); $x_0 = x$; $x = T_{-1}(x)$; $\Delta = 1 - x_0/x$; end while;*
5.   *If $x < b$; $i = i + 1$; $\alpha[i] = x$; $x = S_{-\pi}(x)$; end if;*
6. *end while;*

In the algorithm, all the computed x-values form a strictly increasing sequence. The process continues until the whole interval is spanned and all the zeros are computed. Figure 3.1 shows a graphical example of application of Algorithm 1.

For the case $A'(x) > 0$ an analogous algorithm can be given, but with the zeros generated in decreasing order. For equations with nonmonotonic coefficients $A(x)$, the method can be applied by computing zeros in each subinterval where $A(x)$ is monotonic. As we will see in section 5, this can be easily done for a large set of important special functions (all classical orthogonal polynomials included).

Next, we give a version of the algorithm that is valid for intervals where $A(x)$ is strictly increasing or strictly decreasing and $A(x) > 0$.

ALGORITHM 2 (monotonic and positive $A(x)$ in $[a, b]$).
Input: interval $[a, b]$, $j = sign(A'(x))$, relative error tolerance ϵ
Output: zeros $\alpha[i]$, $i = 1, 2, \ldots$ ($sign(\alpha[i + 1] - \alpha[i]) = -j$)
1. *$x_M = (b + a)/2 - j*(b - a)/2$; $x = x_M$; $i = 0$;*
2. *While $j*(x - x_M) > 0$ and $A(x) > 0$*
3.   *$\Delta = \epsilon + 1$;*
4.   *While ($\Delta > \epsilon$ and $j*(x - x_M) > 0$ and $A(x) > 0$)*
5.   *$x_0 = x$; $x = T_j(x)$; $\Delta = |1 - x/x_0|$;*
6.   *end while;*
7. *If $j*(x - x_M) > 0$ and $A(x) > 0$; $i = i + 1$; $\alpha[i] = x$; $x = S_{j\pi}(x)$; end if;*
8. *end while;*

3.1. The case of the monotonic region $A(x) < 0$. The solutions of second order ODEs $y''(x) + A(x)y(x) = 0$ in intervals where $A(x) < 0$ have, at most, one zero of $y(x)$ or $y'(x)$ in this interval, but not of both functions. This is because $y''(x)y(x) \geq 0$ when $A(x) < 0$. The zeros in the region are isolated zeros and therefore easy to locate and to compute (for instance, using bisection). But to speed up the computation a fourth order FPM can be also considered.
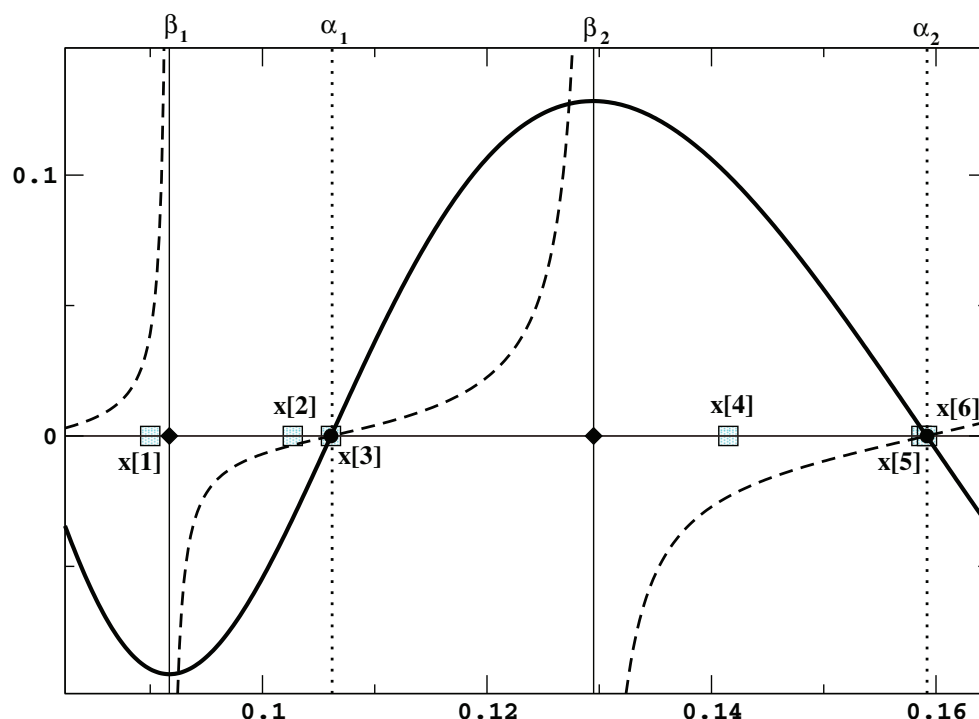
FIG. 3.1. *The function $y(x) = x\sin(1/x)$, solution of $y''(x) + x^{-4}y(x) = 0$, is plotted (solid line) together with the function $h(x) = y(x)/y'(x)$ (dashed line). The computation of the two zeros α_1 and α_2 within four digits of accuracy is illustrated. $x[i]$ is the sequence of increasing values generated by the method. The sequence is the following: $x[1] = 0.09$, $x[2] = T_{-1}(x[1])$, and $x[3] = T_{-1}(x[2]) = 0.10699\ldots \simeq \alpha_1 = (3\pi)^{-1}$. Then, we compute $x[4] = S_{-\pi}(x[3])$, $x[5] = T_{-1}(x[4])$, and $x[5] = T_{-1}(x[5]) = 0.15915\ldots \simeq \alpha_2 = (2\pi)^{-1}$.*

As in section 2, we integrate approximately the Riccati equation for $h(x) = y(x)/y'(x)$. Because now $A(x) < 0$ we take $w(x) = \sqrt{-A(x)}$, and we have

(3.5) $$h'(x) = 1 - (w(x)h(x))^2.$$

By integrating with $W = w(x)$ constant and assuming that $|Wh(x)| < 1$, we obtain

(3.6) $$\frac{1}{W}\tanh^{-1}(Wh(x)) \simeq x - \alpha.$$

This leads to the FPM

(3.7) $$x_{n+1} = \tilde{g}(x_n), \quad \tilde{g}(x) = x - \frac{1}{w(x)}\tanh^{-1}(w(x)h(x)).$$

The method is of fourth order. Indeed,

(3.8) $$\tilde{g}'(x) = \frac{w'(x)}{w(x)^2}\left[\tanh^{-1}(wh) - \frac{wh}{1 - (wh)^2}\right],$$

and, following the ideas of section 2.1, we can easily check that

(3.9) $$\epsilon_{n+1} = \frac{A'(\alpha)}{12}\epsilon_n^4 + \mathcal{O}(\epsilon_n^5).$$

As for (2.9), monotonic convergence can be guaranteed for starting values $x_0 < \alpha$ when $A'(x) < 0$ and for $x_0 > \alpha$ if $A'(x) > 0$.

Usually, the monotonic case $A(x) < 0$ will appear at the extremes of the interval $[a, b]$ where the zeros are sought. In these cases, one can easily combine Algorithm 2 with the fixed point iteration (3.7) in order to compute all the zeros by means of fourth order methods. For example, in the case $A'(x) < 0$ in $[a, b]$ and $A(a) > 0$, $A(b) < 0$, because $A(x)$ is decreasing, one would start by computing the zeros in increasing order in the left of the interval (using Algorithm 2). At some point in the process, an x-value will be reached such that $A(x) < 0$; let us denote this value by x_-. It is easy to prove, by considerations similar to those used for proving monotonic convergence for the iterations (2.9) and (3.2), that if there is a zero α of $y(x)$ such that $A(\alpha) < 0$, then $x_- < \alpha$. In addition, if there is a zero α in $[x_-, b]$, it is necessary that $h(x_-) < 0$, $h(b) > 0$, and $|h(x_-)w(x_-)| < 1$; these necessary conditions are easy to understand by considering that $1/|w(x)|$ is decreasing, that $h(x)$ is increasing when $|h(x)| < 1/|w(x)|$ and decreasing when $|h(x)| > 1/|w(x)|$, and that $h'(\alpha) = 1$. If these necessary conditions are met, then the iteration (3.7) can be used to compute the zero α, if it exists. In case it exists, convergence is monotonic; if it does not exist, the change of sign of $h(x)$ is due to the existence of a zero of $y'(x)$ in (x_-, b); in the latter case, it is easy to prove that the iteration of (3.7) necessarily produces at some step a value x_k such that $|w(x_k)h(x_k)| > 1$.

From the previous discussion, it follows that in order to compute the zeros in intervals where $A(x)$ is monotonic and with a possible change of sign in the interval, a simple modification of Algorithm 2 is enough. The following lines should be added:

   9. *If $A(x) < 0$ and $jh(x) > 0$ and $jh(x_M) < 0$*

   10. $\Delta = \epsilon + 1$;

   11.   *While $(\Delta > \epsilon$ and $|h(x)w(x)| < 1$ and $j(x - x_M) > 0)$*

   12. $x_0 = x$; $x = \tilde{g}(x)$; $\Delta = |1 - x/x_0|$;

   13.   *end while;*

   14.   *If $\Delta < \epsilon$; $i = i + 1$; $\alpha_i = x$; end if;*

   15. *end if;*

3.2. Computation of the zeros of the derivative. Next, we turn to the problem of computing the zeros of $y'(x)$, $y(x)$ being a solution of $y''(x) + A(x)y(x) = 0$.

A fixed point iteration, obtained from the approximate integration of the Riccati equation for $\hat{h}(x) = y'(x)/y(x)$, was considered in [8]. This method for the zeros of $y'(x)$ is "only" of order two. Combined with the DDE methods for the zeros $y(x)$ (also of order two), a method to compute both the zeros of $y(x)$ and $y'(x)$ was obtained. Next, we will see that it is possible to compute the zeros of $y'(x)$ in a way similar to what we have done for the zeros of $y(x)$.

Assuming that $A(x) > 0$, the FPM for the zeros of $y'(x)$ reads [8]

$$(3.10) \qquad x_{n+1} = \bar{g}(x_n), \quad \bar{g}(x) = x + \frac{1}{w(x)} \arctan\left(\frac{1}{wh(x)}\right),$$

where, as for the FPM (2.9), $w(x) = \sqrt{A(x)}$, $h(x) = y(x)/y'(x)$. This iteration also has monotonic convergence properties in the sense of the first two results of Theorem 2.2, but, in contrast to Theorem 2.2, this takes place in the intervals where $h(x)A'(x) < 0$.

As in (3.2), we can modify (3.10) and define new iterations as follows:

(3.11)
$$
\begin{aligned}
x_{n+1} &= \hat{T}_j(x_n), \\
\hat{T}_j(x) &= \begin{cases} x - \dfrac{1}{w(x)} \arctan_j\left(\dfrac{-1}{w(x)h(x)} \right) & \text{if } y(x) \neq 0, \\ x - \dfrac{1}{w(x)} j\dfrac{\pi}{2} & \text{if } y(x) = 0. \end{cases}
\end{aligned}
$$

Then, we have the following result, which is analogous to Theorem 3.1.

THEOREM 3.2. *Let $y(x)$ be a solution of $y''(x) + A(x)y(x) = 0$ with two consecutive zeros of $y'(x)$, β_1, and β_2, such that $A(x) > 0$ in $[\beta_1, \beta_2]$.*

1. *If $A'(x) > 0$ in (β_1, β_2), then the sequence (3.11) converges monotonically to β_1 for any $x_0 \in (\beta_1, \beta_2]$.*
2. *If $A'(x) < 0$ in (β_1, β_2), then the sequence (3.11) converges monotonically to β_2 for any $x_0 \in [\beta_1, \beta_2)$.*

The order of convergence is two.

The proof follows the reasoning of that of Theorem 3.1. The most important difference is that the method is of order two only.

For the oscillatory region $A(x) > 0$, an algorithm similar to Algorithm 1 can be used to compute the zeros of $y'(x)$, but using the iterations $\hat{T}_j$. For the monotonic region $A'(x) < 0$, the zero of $y'(x)$ (only one at most) can be computed using (3.10), but with $\arctan(1/(wh))$ replaced by $-\tanh^{-1}(1/(wh))$ (see [8, Thm. 3.14]).

Because the computations of the zeros of $y(x)$ and $y'(x)$ are both carried out in the same direction, it is possible to write a simple algorithm to compute zeros of $y(x)$ and $y'(x)$ in a row. The resulting algorithm is far simpler than the algorithm given in [8] but also more efficient (particularly when computing the zeros).

We observe, as discussed in [8], that for equations $v''(x) + \tilde{B}(x)v'(x) + \tilde{A}(x)v(x) = 0$ one cannot transform to normal form by a change of function (2.3) when the zeros of $y'(x)$ are to be computed, because the zeros of the derivative would change with the change of function. Instead, the change of variable

(3.12)
$$
z(x) = \int^x \exp\left(-\int^\zeta B(t)dt \right) d\zeta
$$

can be considered. As discussed in [8], this change is simple in many instances.

In principle it is also possible to construct a fourth order method for the zeros of $y'(x)$ by using the second order ODE satisfied by $v(x) = y'(x)$ (differentiating the ODE and eliminating $y(x)$). However, the transformation to normal form with a change of variable (3.12) or function (2.3) usually leads to a hard problem: either the change of variable is not analytically invertible, or it is difficult to analyze the monotonicity properties of the coefficient of the resulting equation in normal form.

Here we leave the discussion on the computation of the zeros of $y'(x)$ and turn to the more important problem of computing zeros. Further details will be given in a future publication [9] describing specific software implementing these methods.

4. Nonlocal behavior of the algorithm. Because the method (3.2) is of fourth order, convergence is extremely fast if a starting value close to a zero is available. However, because the zeros are computed without using a priori estimations, it is important that few steps are required before a value close to the zero is reached. Figure 3.1 gives an example in which two iterations are enough for this purpose. Such good nonlocal behavior is far from being an isolated case, as we next explain.

We establish the following criterion in order to quantify the nonlocal behavior.

DEFINITION 4.1. *Let $A(x)$ be a positive and monotonic function and $y(x)$ a solution of $y''(x) + A(x)y(x) = 0$. Let α_1 and α_2, $\alpha_1 < \alpha_2$, be two consecutive zeros of $y(x)$ and β be the only zero of $y'(x)$ in the interval (α_1, α_2). We will say that $T_j(x)$ has good nonlocal behavior in (α_1, α_2) if one of the following two conditions holds:*

    1. *$T_{+1}(\alpha_2) \in (\alpha_1, \beta)$ when $A'(x) > 0$.*
    2. *$T_{-1}(\alpha_1) \in (\beta, \alpha_2)$ when $A'(x) < 0$.*

Let us, for instance, consider the second case in the definition. This criterion means that, after the zero α_1 has been computed, the next iteration, $T_{-1}(\alpha_1)$, gives a value which is beyond the zero of $y'(x)$ between α_1 and α_2 (which is the next zero of $y(x)$ to be computed). In some sense, this means that the first iteration is already "half way there." In Figure 3.1 there is good nonlocal behavior: after $x[3] \approx \alpha_1$ has been computed, the next iteration gives a value beyond the zero of $y'(x)$ in (α_1, α_2).

It is easy to find a sufficient condition for good nonlocal behavior.

THEOREM 4.2. *Let $A(x)$, $y(x)$, α_1, α_2, and β be as in Definition 4.1. Let A_M be the maximum value of $A(x)$ in $[\alpha_1, \alpha_2]$. Then, if $A_M/A(\beta) < 4$, the iteration $T_j(x)$ has good nonlocal behavior in (α_1, α_2).*

Proof. Take the case $A'(x) < 0$. Because by Lemma 2.1 $\beta - \alpha_1 < \pi/(2\sqrt{A(\beta)})$, we have that $T_{-1}(\alpha_1) = \alpha_1 + \pi/\sqrt{A(\alpha_1)} > \beta$ if $A(\alpha_1)/A(\beta) < 4$, and $A_M = A(\alpha_1)$. On the other hand, $T_{-1}(\alpha_1) < \alpha_2$ because of Theorem 3.1.   □

Instead of (4.2), it will be easier to deal with a more stringent condition.

COROLLARY 4.3. *Let $A(x)$ be positive and monotonic between two consecutive zeros $\alpha_1 < \alpha_2$. Then, if $1/4 < A(\alpha_2)/A(\alpha_1) < 4$, the iteration $T_j(x)$ has good nonlocal behavior in (α_1, α_2).*

It is not surprising that the algorithm behaves better as the ratios $A(\alpha_{k+1})/A(\alpha_k)$ are close to 1, because if $A(\alpha_{k+1})/A(\alpha_k) = 1$ and $A(x)$ is monotonic, then $A(x)$ is constant, and the method is automatically exact (only one iteration for each root needed).

4.1. Nonlocal behavior for the equation $y''(x) + x^{-m}y(x) = 0$. The condition for good nonlocal behavior (Corollary 4.3) is met quite generally. Let us observe that if, for instance, $A(x)$ increases as x increases, on account of Sturm's theorem (see, for instance, [2, Thm. 3]), the zeros tend to come closer together as x increases, and this acts as a counterweight to the fact that $A(x)$ increases. This is why the condition of Corollary 4.3 is satisfied more generally than one might naively expect.

As an illustration of the good nonlocal properties of the method, we consider the relatively simple but important example of ODEs

$$(4.1) \qquad \ddot{y}(z) + \lambda z^{-m}y(z) = 0, \quad \lambda > 0, \ z > 0.$$

Let us notice that, except for $m = 2$, it is sufficient to consider the equation

$$(4.2) \qquad y''(x) + x^{-m}y(x) = 0$$

because the change $z = \lambda^{1/(m-2)}x$ transforms (4.1) into (4.2).

We start with the case $m = 2$ (the Cauchy–Euler equation).

THEOREM 4.4. *Let $y(x)$ be a solution of*

$$(4.3) \qquad y''(x) + A(x)y(x) = 0, \quad A(x) = \frac{\nu^2 + 1/4}{x^2}.$$

If $\nu \neq 0$, then $y(x)$ has infinitely many zeros in $(0, a)$ and $(a, +\infty)$ for any $a > 0$.

Let $\{\alpha_k\}$ be the sequence of zeros of $y(x)$ arranged in increasing order; then

$$(4.4) \qquad A(\alpha_{k+1})/A(\alpha_k) = e^{-2\pi/|\nu|},$$

and the condition for good nonlocal behavior (Corollary 4.3*) holds when $\nu > \pi/\log(2)$.*

Proof. With the change of variables $x = e^z$, (4.3) transforms into an equation with constant coefficients. Then we find the general solution

$$(4.5) \qquad y(x) = A\sqrt{x}\sin(|\nu|\log(x) + \phi),$$

and the results follow easily. □

Notice that when the condition for good nonlocal behavior is violated, it fails to hold for all the zeros. Theorem 4.4 explains the bad small parameter behavior of some of the examples considered in section 5 (Bessel functions of imaginary order and conical functions). Not surprisingly, exponential changes of variable eliminate this problem.

Next, we consider (4.2) for $m \neq 2$. In contrast to the case $m = 2$, the condition for good nonlocal behavior holds asymptotically. This means that the condition could be violated for a finite number zeros only (usually a very low number; see Corollary 4.7 and the subsequent discussion).

In the next theorem we follow the notation of [6] for the zeros of Bessel functions: $j_{\mu,\kappa}$, $\kappa \in (k-1, k]$, will denote the kth positive zero of the Bessel function $\mathcal{C}_\mu(x, \gamma) = \cos\gamma J_\mu(x) - \sin\gamma Y_\mu(x)$, with $\gamma = (k - \kappa)\pi \in [0, \pi)$.

THEOREM 4.5. *Let $y(x)$ be a solution of*

$$(4.6) \qquad y''(x) + A(x)y(x) = 0, \quad A(x) = x^{-m}, m \neq 2;$$

then, given any $a > 0$, the solution has an infinite number of zeros in $(0, a)$ if $m > 2$ and in $(a, +\infty)$ if $m < 2$ (but no solution has an infinite number of zeros in both intervals).

Let α_k, $k \in \mathbb{N}$, be the zeros of $y(x)$ with the ordering $\alpha_k < \alpha_{k+1}$ if $m < 2$ and $\alpha_k > \alpha_{k+1}$ if $m < 2$. Then the ratio $A(\alpha_{k+1})/A(\alpha_k)$ is monotonic as a function of k and $\lim_{k \to +\infty} A(\alpha_{k+1})/A(\alpha_k) = 1$.

Proof. It is a straightforward matter to verify that with the change of variable $z(x) = x^{1-m/2}/|1-m/2|$ the function $Y(z) = z^{m/(2m-4)}y(x(z))$, $y(x)$ being a solution of (4.6), satisfies the equation

$$(4.7) \qquad \ddot{Y}(z) + \Omega(z)Y(z) = 0, \quad \Omega(z) = 1 - \frac{\nu^2 - 1/4}{z^2}, \quad \nu = (m-2)^{-1}.$$

The general solutions can be expressed in terms of Bessel functions as $Y(z) = \sqrt{z}\mathcal{C}_{|\nu|}(z, \gamma) = \sqrt{z}(\cos\gamma J_{|\nu|}(z) - \sin\gamma Y_{|\nu|}(z))$. We can restrict our attention to positive orders ν because (4.7) does not depend on the sign of ν and γ is some unspecified angle.

The kth positive zero of any solution of (4.7) can be written as $j_{|\nu|,\kappa}$, $\kappa = k - \gamma/\pi$, for some $\gamma \in [0, \pi)$, and, undoing the change of variables, we have

$$(4.8) \qquad \alpha_k = \left(\frac{j_{|\nu|,\kappa}}{2|\nu|}\right)^{-2\nu}, \quad \nu = (m-2)^{-1}.$$

Because Bessel functions have an infinite number of positive real zeros and the number of zeros in intervals $(0, a)$, $a > 0$, is finite, the assertion about the distribution

of zeros follows from (4.8) and known properties of zeros of Bessel functions. In addition, using (4.8), we find

$$(4.9) \qquad \frac{A(\alpha_{k+1})}{A(\alpha_k)} = \left(\frac{j_{|\nu|,\kappa+1}}{j_{|\nu|,\kappa}}\right)^{2(1+2\nu)}, \quad \kappa \in (k-1,k],$$

and the monotonicity result is a consequence of (4.9) and the fact that

$$(4.10) \qquad 1 < j_{\mu,\kappa+2}/j_{\mu,\kappa+1} < j_{\mu,\kappa+1}/j_{\mu,\kappa}, \quad \kappa \geq 0,$$

for any real μ (see [2, Thm. 22]). On the other hand, because $j_{\nu,k} \to +\infty$ and $j_{\nu,k+1} - j_{\nu,k} \to \pi$ as $k \to +\infty$, we have $\lim_{k\to+\infty} A(\alpha_{k+1})/A(\alpha_k) = 1$. $\quad \square$

Remark 2. Theorem 4.5 proves that the greatest deviation of $A(\alpha_{k+1})/A(\alpha_k)$ from 1 occurs for the smallest k (the smallest zeros if $m < 2$ and the largest ones if $m > 2$) and that the behavior as $k \to +\infty$ is optimal. This means that the hardest zeros to compute with Algorithm 2 should be the last computed zeros when $m < 0$ or $m > 2$ and the first zeros when $0 < m < 2$. Indeed, and as explained in section 5, these extreme zeros usually need one additional iteration compared to the rest.

Next we give an operative condition for good nonlocal behavior. For this, the following result is needed.

LEMMA 4.6. $j_{\nu,\kappa+\epsilon}/j_{\nu,\kappa}$, $\kappa > 0$, *is a decreasing function of κ for any $\epsilon > 0$.*[1]

Proof. This result is proved by using the relation

$$(4.11) \qquad D_\kappa(\log(j_{\nu,\kappa})) = \frac{\pi^2}{2}(J_\nu(j_{\nu,\kappa})^2 + Y_\nu(j_{\nu,\kappa})^2), \quad \kappa > 0$$

(see [5, 17]), and considering that $j_{\nu,\kappa}$ is an increasing function of κ and that $J_\nu(x)^2 + Y_\nu(x)^2$ is a decreasing function of x (which is proved using the Nicholson formula [23, p. 444]).[2] $\quad \square$

With this, and considering (4.9), it is immediate to prove the following corollary.

COROLLARY 4.7. *Let $p \geq 2$, $p \in \mathbb{N}$, be such that*

$$(4.12) \qquad \left(\frac{j_{|\nu|,p}}{j_{|\nu|,p-1}}\right)^{|1+2\nu|} < 2, \quad \nu = (m-2)^{-1};$$

then, for any $k \geq p$, the iteration (3.2) for the equation $y''(x) + x^{-m}y(x) = 0$ has good nonlocal behavior in the intervals limited by α_k and α_{k+1}.

A numerical test of (4.12) shows that the inequality is satisfied for $p = 2$ if $m \in (-12, 1.05)$. This proves good nonlocal behavior for any solution of important equations such as the Airy equation ($m = -1$) and the Weber parabolic cylinder function equation ($m = -2$) except, possibly, for the first zero. Of course, the larger the p, the larger the m-intervals; for $p = 3$, (4.12) is satisfied if $m \leq 1.2$ or $m \geq 2.4$. The actual situation is better than (4.12) predicts, and, for instance, Figure 3.1 shows an example of a solution for $m = 4$ for which good nonlocal behavior takes place for all the zeros. Notice that the condition for good nonlocal behavior is given by Theorem 4.2 but that we have used the more restrictive condition of Corollary 4.3 for simplicity.

---

[1]It is also a decreasing function of ν, as can be checked by using the relation [6] $D_\nu(\log(j_{\nu,\kappa})) = 2\int_0^{+\infty} K_0(2j_{\nu,\kappa}\sinh t)e^{-2\nu t}dt$, the fact that $j_{\nu,\kappa}$ is an increasing function of κ, and the decrease of the modified Bessel function $K_0(x)$ as a function of x.

[2]The author thanks Prof. M. E. Muldoon for pointing out (4.11) as a way to prove this lemma.

5. Applications. The algorithm to compute zeros is straightforward to use when it is possible to compute the regions of monotonicity of the coefficient $A(x)$. As we show next, this can be done easily for a large number of special functions, including all classical orthogonal polynomials. Therefore, the method can be used for a fast and very accurate computation of nodes of Gaussian quadratures (and also weights; see, for instance, [22, Thm. 6.5]) as well as for the computation of zeros of many other important special functions. As we will see, in some cases it will be useful to consider a Liouville transformation to obtain an alternative equation with simpler monotonicity properties or to improve the speed of convergence. A Liouville transformation of an equation in normal form is a change of variables followed by a transformation to normal form using (2.2)–(2.4) (see, for instance, [18, p. 191]).

We tested the method using Maple. More efficient function evaluation methods are usually available, but Maple is a convenient platform for testing the algorithm for as wide a set of differential equations as possible. We refer the reader to [10, Chap. 12] for a description of efficient algorithms to compute some of the functions we discuss next. In particular, for functions for which the matrix eigenvalue methods can be applied (orthogonal polynomials and minimal solutions of three-term recurrence relations) the ratio $h(x) = y(x)/y'(x)$ can be computed using the same information as the matrix methods, namely, the coefficients of a three-term recurrence relation. But, as happens with DDE methods [8, sect. 4], the method here described is not limited to these solutions.

The general claim for the examples we discuss next is that the number of iterations needed for 100-digit accuracy is, with few exceptions, 4 or 5 (counting the extra iteration needed for checking accuracy). For 16-digit accuracy we need one or two fewer iterations. As otherwise stated, the examples will satisfy this general claim. In some important cases (Jacobi polynomials), the performance is even better.

5.1. Three differential equations with trivial solutions. First we test the method on three differential equations with elementary solutions. These examples confirm the behavior described in section 4.1 for the equation $y''(x) + x^{-m}y(x) = 0$ and show that good nonlocal behavior is a useful efficiency indicator.

The ODEs $y''(x) + A(x)y(x) = 0$ and general solutions are as follows:
1. $A(x) = x^{-4}$. General solution: $y(x) = Cx\sin(1/x + \phi)$.
2. $A(x) = (16x + 3)/(16x^2)$. General solution: $y(x) = Cx^{1/4}\sin(2\sqrt{x} + \phi)$.
3. $A(x) = (\nu^2 + 1/4)/x^2$. General solution: $y(x) = C\sqrt{x}\sin(|\nu|\log x + \phi)$.

The first case corresponds to $m = 4$. It is observed, as expected (see Remark 2 following Theorem 4.5), that the most expensive zeros are the last computed ones. In this relatively unfavorable case, for 100-digit accuracy the last and largest zero for the solution $y(x) = x\sin(1/x)$ requires 6 iterations, the next 16 zeros 5 and the rest 4.

The second case corresponds to $m = 1$ (for large x), and, as expected, the most expensive zeros are the last zeros computed, which are the smallest. For example, the 9 smallest zeros of $y(x) = x^{1/4}\sin(2\sqrt{x})$ require 5 iterations and the rest 4 or less.

Finally, the third case corresponds to the Cauchy–Euler equation ($m = 2$), which is the worst-case scenario, particularly for small $|\nu|$. The behavior of the algorithm is expected to be uniform for all the zeros and worsening as $|\nu|$ becomes small (Theorem 4.4). For instance, when $\nu = 0.2$, we typically need 13 or 14 iterations for each zero. As ν increases, the situation improves, and 5 iterations are enough for $\nu = 3$.

Of course, the zeros of the Cauchy–Euler equation are best computed by applying the change of variables $x = e^z$ and solving the resulting trivial equation. As we will see, exponential transformations also improve the performance for some special function

examples which behave like a Cauchy–Euler equation for small or large x (Bessel and modified Bessel functions of imaginary orders for small x, and conical functions for large x). The worst-case scenario for the method is solved with simple changes of variable.

5.2. $A(x)$ a polynomial, $\deg(A(x)) \leq 2$. Any solution of the equation $y''(x) + A(x)y(x) = 0$ can be written in terms of the solutions of one the following three cases, up to linear changes of variable:

1. $A(x) = x$. Standard solutions: $\mathrm{Ai}(-x)$ and $\mathrm{Bi}(-x)$ [1, sect. 10.4].
2. $A(x) = x^2/4 - a$. Standard solutions: $W(a, \pm x)$ [1, Chap. 19].
3. $A(x) = -(x^2/4 + a)$. Solutions: $U(a, x)$ and $V(a, x)$ [1, Chap. 19].

Without loss of generality, we consider positive real zeros.

Maple computes the Airy functions $\mathrm{Ai}(-x)$ and $\mathrm{Bi}(-x)$ and the parabolic cylinder functions (PCFs) $U(a, x)$ and $V(a, x)$ (and, in particular, Hermite polynomials), but not the PCFs $W(a, x)$, which we compute in terms of confluent hypergeometric functions of complex arguments [1, sect. 19.25].

The Airy functions correspond to the case $m = -1$ considered in section 4.1. The $W(a, \pm x)$ case corresponds to the case $m = -2$ for large x. As explained in section 4.1, these cases are expected to have good nonlocal behavior. Not surprisingly, the general claim on the number of iterations applies.

The third case is not related to the equations discussed in section 4.1, and the solutions have a finite number of zeros. Observe that, as $|a|$ becomes larger with $a < 0$, we have an almost constant positive $A(x)$ for small x, which is favorable for the method. Indeed, it is observed that as a becomes more negative, the performance improves. But for small $|a|$ the performance is already good (for instance, five iterations for $a = -3$).

5.3. $q(x) = x^2 A(x)$ a quadratic polynomial. These are functions of confluent hypergeometric type. Without loss of generality, we consider positive real zeros.

We consider the equation

$$(5.1) \qquad y''(x) + \left[-\epsilon_1^2 - 2\frac{\eta}{x} + \frac{1/4 - \epsilon_2^2 \nu^2}{x^2} \right] y(x) = 0;$$

ϵ_1 and ϵ_2 may take the values 1 or i (imaginary unit), and ν and η are real.

Any solution of (5.1) has an infinite number of real zeros in $(a, +\infty)$ for any $a > 0$ when $\epsilon_1 = i$ and an infinite number of real zeros in $(0, a)$ for any $a > 0$ when $\epsilon_2 = i$. On the other hand, if $\epsilon_1 = \epsilon_2 = 1$, the solutions have a finite number of zeros.

The coefficient $A(x)$ has one extremum for $x > 0$ at most, located at $x_e = (1/4 - \epsilon_2^2 \nu^2)/\eta$. Therefore, the monotonicity properties are very simple, and the zeros can be easily computed with the algorithms described before.

It is straightforward to check, using [1, Eq. 13.1.1], that a solution of (5.1) is

$$(5.2) \ \ y_{\epsilon_1, \epsilon_2}(\eta, \nu, x) = \sqrt{x}\, x^{\epsilon_2 \nu} e^{-\epsilon_1 x}\, {}_1\mathrm{F}_1\left(\eta/\epsilon_1 + \epsilon_2 \nu + \frac{1}{2}; 2\epsilon_2 \nu + 1; 2\epsilon_1 x \right), \quad x > 0.$$

We test the algorithms using the solutions (5.2), which for $\epsilon_2 = 1$ are real solutions, as can be checked using the reflection formula [1, Eq. 13.1.27]. Contrarily, (5.2) is a complex solution if $\epsilon_2 = i$, and it is obvious that the complex conjugate is also a solution; therefore, the real and imaginary parts of (5.2) are real solutions of (5.1). We test the algorithms with these real solutions.

As particular cases, we have the Laguerre case when $\epsilon_1 = \epsilon_2 = 1$. Equation (5.2) is related to Laguerre functions (which are polynomials for integer n) as follows:

$$(5.3) \qquad y_{1,1}(-n - (\alpha+1)/2; \alpha/2; x/2) = \frac{n!}{(\alpha+1)_n} x^{(\alpha+1)/2} e^{-x/2} L_n^{(\alpha)}(x).$$

When $\epsilon_1 = i$, $\epsilon_2 = 1$, the real solution (5.2) is related to the regular Coulomb wave function [1, Eq. 14.1.3].

For cases different from the Laguerre case, particular solutions for $\eta = 0$ are available in Maple in terms of Bessel functions of real or imaginary orders [4]. For $\epsilon_1 = i$ and $\epsilon_2 = 1$ two real solutions are $\sqrt{x}J_\nu(x)$ and $\sqrt{x}Y_\nu(x)$. For $\epsilon_1 = 1$ and $\epsilon_2 = i$, the solutions can be expressed in terms of the real and imaginary parts of $\sqrt{x}I_{i\nu}(x)$ ($I_\mu(x)$ is the modified Bessel function of the first kind). For $\epsilon_1 = i$ and $\epsilon_2 = i$, two real solutions are the real and imaginary parts of $\sqrt{x}J_{i\nu}(x)$.

For all these test functions, it is observed that the claim on the number of iterations holds, but with two types of exceptions.

First, for $\epsilon_2 = i$ the coefficient $A(x)$ is such that $A(x) \simeq (\nu^2 + 1/4)/x^2$ as $x \to 0^+$; the equation behaves like a Cauchy–Euler equation and, as expected, for small ν the performance worsens. This is solved by Liouville-transforming the equation with the change $x = e^z$. For the transformed equation, the maximal number of iterations for $|\nu| < 2$ is 3.

Second, in the Laguerre case (5.3), $A(x)$ is strictly decreasing when $|\alpha| < 1$, and the algorithm to compute the positive zeros starts with small x (therefore, close to the singularity of $A(x)$). It is convenient to bound the search for zeros and consider search intervals $[a, b]$ with a not too close to $x = 0$. Using $a = (1 + \alpha)/n$ when $|\alpha| \le 1$, $\alpha > -1$ [13], the smallest zero is computed with four or fewer iterations. It is not required that a value b be fixed, but taking $b = 2(2n + \alpha + 1)$ is enough to guarantee that all the zeros of the Laguerre polynomial are computed (for a finer bound, see [15]).

Comparing the performance of the method with the DDE methods to compute zeros introduced in [20, 8], it is observed that the new method generally reaches 100-digit accuracy for the same number of iterations for which the DDE methods gives 15 digits (see [8, 7] for numerical illustrations of the DDE method). In addition, the number of iterations needed is more homogeneous for the new method and does not increase sharply for the extreme zeros. On the other hand, the DDE methods are not applicable for the cases $\epsilon_1 = 1$, $\epsilon_2 = i$, and $\epsilon_1 = \epsilon_2 = i$.

5.4. Functions of Gauss hypergeometric type. We concentrate on two important functions: Jacobi polynomials and conical functions.

5.4.1. Jacobi polynomials. Jacobi functions $P_n^{(\alpha,\beta)}(x)$, $x \in (-1, 1)$, are related to Gauss hypergeometric functions [1, Eq. 15.4.6]; they are polynomials when $n \in \mathbb{N}$. Particular examples are Legendre ($\alpha = \beta = 0$), Chebyshev ($|\alpha| = |\beta| = 1/2$), and Gegenbauer ($\alpha = \beta = \lambda - 1/2$) polynomials, as well as the associated Legendre functions $P_n^m(x)$, which are Jacobi polynomials $P_n^{(-m,m)}(x)$ up to a trivial factor without zeros in $(-1, 1)$.

Transforming the Jacobi equation [1, Eq. 22.6.1] to normal form, we obtain an equation with a coefficient $A(x)$ with rather complicated monotonicity properties [3]. It is convenient to consider the Liouville transformation with change of variable $x = \cos z$, which gives a transformed equation in normal form with a coefficient with

simple monotonicity behavior (see [2, 3]). It is easy to check that the function

$$(5.4) \qquad Y(z) = \left(\sin\frac{z}{2}\right)^{\alpha+1/2}\left(\cos\frac{z}{2}\right)^{\beta+1/2} P_n^{(\alpha,\beta)}(\cos z)$$

is a solution of an equation in normal form $\ddot{Y}(z) + \Omega(z)Y(z) = 0$ with coefficient

$$(5.5) \qquad \Omega(z) = \frac{1}{4}\left[(2n+\alpha+\beta+1)^2 + \frac{1/4-\alpha^2}{\sin^2(z/2)} + \frac{1/4-\beta^2}{\cos^2(z/2)}\right].$$

The function $\Omega(z)$ either has only one relative extremum for $z \in (0,\pi)$, located at $z_e = \arccos(1 - 2\lambda_\alpha/(\lambda_\beta + \lambda_\alpha))$, $\lambda_\mu = \sqrt{|1/4 - \mu^2|}$, or is monotonic.

The new variable z is preferable to x, because the monotonicity properties are easier, but also because the convergence is faster. Only three–four iterations of (2.9) are required in order to compute the zeros with more than 100-digit accuracy. Observe that $\Omega(z)$ is constant when $|\alpha| = |\beta| = 1/2$ (the Chebyshev cases), and then the method is exact with only one function evaluation per root. Also, when $L = 2n+\alpha+\beta+1$ becomes large, $\Omega(z)$ is approximately constant, particularly close to $z = \pi/2$.

In order to compute all the zeros in $(-1,1)$, one should consider a search interval $[-1+\epsilon, 1+\epsilon]$, with ϵ a small positive number. The performance of the method is the same, irrespective of how small ϵ is taken, except when the relative extremum of $\Omega(z)$ is a minimum, which is the case $|\alpha| < 1/2$, $|\beta| < 1/2$, or when it is monotonic ($|\alpha| < 1/2$ or $|\beta| < 1/2$ but not both). In these cases (as happened for Laguerre polynomials when $|\alpha| \le 1$), bounds for the smallest and largest zeros are convenient, because otherwise the algorithm would start close to one or both singularities of the differential equation. Simple and effective bounds are given in [15, 16]. With these bounds, the extreme zeros are computed as efficiently as the rest.

5.4.2. Conical functions. These are solutions of the differential equation

$$y''(x) + \frac{2x}{x^2-1}y'(x) + \left[\frac{1/4+\tau^2 - m^2/(x^2-1)}{x^2-1}\right]y(x) = 0, \quad x > 1.$$

One of their solutions is the Legendre function $P_{-1/2+i\tau}^m(x)$. After transforming to normal form, the $A(x)$ coefficient of the ODE shows simple monotonicity properties (one extremum at most), and the problem is tractable in the original variable. However, $A(x) \sim (\tau^2 + 1/4)/x^2$ for large x, and an exponential change of variables is convenient, particularly for small τ.

Considering the change of variables $x = \cosh z$, we see that the function $Y(z) = \sqrt{\sinh z}P_{-1/2+i\tau}^m(\cosh z)$ satisfies the differential equation $\ddot{Y}(z) + \Omega(z)Y(z) = 0$ with

$$(5.6) \qquad \Omega(z) = \tau^2 - \frac{m^2 - 1/4}{\sinh^2 z}.$$

The coefficient $\Omega(z)$ is monotonically increasing for $m > 1/2$, monotonically decreasing for $m < 1/2$, and constant for $m = 1/2$.

In the new variable z, the general claim on the number of iterations holds, and the behavior of the algorithm improves for m close to $1/2$, for small τ or for large z.

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