

# ON THE NUMERICAL CALCULATION OF THE ROOTS OF SPECIAL FUNCTIONS SATISFYING SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

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**Abstract.** We describe a method for calculating the roots of special functions satisfying second order ordinary differential equations. It exploits the recent observation that the solutions of equations of this type can be represented via nonoscillatory phase functions, even in the high-frequency regime. Our approach requires  $\mathcal{O}(1)$  operations per root and achieves near machine precision accuracy. Moreover, despite its great generality, our approach is competitive with (and in many cases, faster than) specialized, state-of-the-art methods for the construction of Gaussian quadrature rules of large orders when it used in such a capacity. The performance of the scheme is illustrated with several numerical experiments.

**Key words.** Special functions, fast algorithms, quadrature

**AMS subject classifications.** 65D32, 33C45

Special functions satisfying second order differential equations

$$y''(t) + q(t)y(t) = 0 \quad \text{for all } -\infty < a \leq t \leq b < \infty, \quad (1)$$

where  $q$  is smooth and positive, are ubiquitous in mathematical physics, and their roots play a number of roles. Among other things, they are related to the resonances in mechanical and electromagnetic systems, arise in quantum mechanical calculations, and are the nodes of Gaussian quadrature formulas.

Their role as the nodes of Gaussian quadrature formulas motivates much of the interest in the numerical computation of the roots of special function defined by equations of the form (1). Every family of classical orthogonal polynomials — Legendre polynomials, Hermite polynomials, Laguerre polynomials, etc. — is associated with a nonnegative weight function  $w$  and a collection of Gaussian quadrature rules, one for each positive integer  $n$ , of the form

$$\int_a^b \varphi(t)w(t) dt \approx \sum_{j=1}^n \varphi(t_j)w_j. \quad (2)$$

The Gaussian quadrature rule (2) is exact when  $\varphi$  is a polynomial of degree less than  $2n$ . The nodes  $t_1, \dots, t_n$  are the roots of a polynomial  $p$  of degree  $n$  that satisfies an equation of the form (1), and, at least in the case of the classical orthogonal polynomials, the weights  $w_1, \dots, w_n$  can be calculated from the values of the derivatives of  $p$  at the nodes  $t_1, \dots, t_n$ .

Many schemes for the numerical computation of the nodes  $t_1, \dots, t_n$  and weights  $w_1, \dots, w_n$  of the rule (2) are based on the observation that classical orthogonal polynomials also satisfy three-term recurrence relations. Using such a recurrence relation to compute Newton iterates which converge to the roots of an orthogonal polynomial yields an  $\mathcal{O}(n^2)$  method for the computation of an  $n$ -point Gaussian quadrature rule. The Golub-Welsch algorithm [16] exploits the connection between three-term recurrence relations and the eigenvalues of symmetric tridiagonal matrices in order to calculate the nodes of an  $n$ -point Gaussian quadrature formula in  $\mathcal{O}(n \log(n))$  operations; it requires  $\mathcal{O}(n^2)$  operations in order to compute both the nodes and weights.

In the last decade, several  $\mathcal{O}(n)$  methods for the calculation of  $n$ -point Gaussian quadrature rules have been proposed. In [4], Newton's method is combined with a scheme, based on asymptotic formulas, for evaluating Legendre polynomials of arbitrary orders and arguments in  $\mathcal{O}(1)$  operations. A similar approach is taken in [20], in which asymptotic formulas for Jacobi polynomials are used to evaluate Newton iterates which converge to the nodes of Gauss-Jacobi quadrature rules. In [34], the approach of [20] is applied to construct Gauss-Hermite quadrature rules and Gaussian quadrature rules for weight functions of the form  $\exp(-V(x))$ , where  $V$  is a polynomial which grows at infinity. The asymptotic formulas used in the construction of the later formulas are derived using Riemann-Hilbert techniques. Asymptotic formulas which approximate the nodes and weights of Gauss-Legendre quadrature rules with double precision accuracy are developed in [3]. Newton's method can be used to refine these approximations if greater accuracy is required, but, in most cases, the asymptotic formulas of [3] allow one to dispense with iterative methods entirely. The scheme of [30] uses a rapidly convergent fixed point method to calculate the roots of solutions of quite general

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second order differential equations of the form (1). Unlike Newton’s method, the fixed point scheme of [30] is guaranteed to converge. This approach has the disadvantage, though, that the regions of monotonicity of the coefficient  $q$  must be explicitly known. The schemes of [3, 4, 20, 34, 30] all have the property that any particular quadrature node and its corresponding weight can be calculated independently of the others, making them suitable for parallelization.

The Glaser-Liu-Rokhlin method [14] combines the Prüfer transform with the classical Taylor series method for the solution of ordinary differential equations. It computes  $n$  roots in  $\mathcal{O}(n)$  operations and is more general than the schemes [3, 4, 20] in that it applies to special functions defined by second order differential equations of the form

$$r_0(t)y''(t) + p_0(t)y'(t) + q_0(t)y(t) = 0, \quad (3)$$

where  $p_0$ ,  $q_0$  and  $r_0$  are polynomials of degree less than or equal to two. This class includes the classical orthogonal polynomials, Bessel functions, prolate spheroidal wave functions, etc. The Glaser-Liu-Rokhlin algorithm does, however, suffer from several disadvantages. It is typically slower than the methods discussed above, and is unsuitable for parallel implementation since the roots must be computed in sequential order (that is, the computation of the  $(n + 1)^{st}$  root can only proceed once the  $n^{th}$  root has been obtained). Moreover, some precision is lost when the Glaser-Liu-Rokhlin technique is used to compute the weights of a Gaussian quadrature rule of large order (see [4] and [20] for discussions of this issue).

Here, we describe a fast and highly accurate algorithm for calculating the roots of special functions which applies in even greater generality than the Glaser-Liu-Rokhlin method. Indeed, it can be used to compute the roots of a solution of an equation of the form (1) as long as  $q$  is a nonoscillatory function which is positive and analytic on the interior of the interval  $[a, b]$  ( $q$  can have poles, branch cuts or zeros at the endpoints  $a$  and  $b$ ). Of course, the ostensibly more general second order linear ordinary differential equation (3) can be easily transformed into the form (1) (see, for instance, [9]), and assuming that the coefficients  $r_0$ ,  $p_0$  and  $q_0$  are nonoscillatory, the algorithm of this paper can be brought to bear on the resulting equation. Despite its great generality, our approach is competitive with the specialized algorithm of [3] for the computation of Gauss-Legendre quadrature rules of large orders, and considerably faster than the specialized approach of [20] for the computation of Gauss-Jacobi quadrature rules of large orders. See the experiments of Sections 5.2 and 5.3 for timings. See also Section 5.4, where the algorithm of this paper is used to compute generalized Gauss-Laguerre quadrature rules.

Our approach exploits the fact that when the coefficient  $q$  in (1) is nonoscillatory, solutions of the equation (1) can be represented to high accuracy via a nonoscillatory phase function, even when the magnitude of  $q$  is large. Of course, the solutions of (1) are highly oscillatory when magnitude of  $q$  is large (this follows from the Sturm comparison theorem). A smooth function  $\alpha : [a, b] \rightarrow \mathbb{R}$  is a phase function for Equation (1) if  $\alpha'$  is positive on  $[a, b]$  and the pair of functions  $u, v$  defined by the formulas

$$u(t) = \frac{\cos(\alpha(t))}{\sqrt{\alpha'(t)}} \quad (4)$$

and

$$v(t) = \frac{\sin(\alpha(t))}{\sqrt{\alpha'(t)}} \quad (5)$$

form a basis in the space of solutions of (1). Phase functions play a major role in the theories of special functions and global transformations of ordinary differential equations [5, 27, 28, 1], and are the basis of many numerical algorithms for the evaluation of special functions (see [31, 15, 22] for representative examples).

When  $q$  is large in magnitude, most phase functions for (1) are highly oscillatory (see Formula (23) in Section 1 and the discussion with accompanies it). However, it has long been known that certain second order differential equations — such Bessel’s equation and Chebyshev’s equation — admit nonoscillatory phase functions [22]. In [21] and [7], it is shown that, in fact, essentially all equations of the form (1), where  $q$  is positive and nonoscillatory, admit a nonoscillatory phase function  $\alpha$  which represents solutions of (1) with high accuracy. The function  $\alpha$  is nonoscillatory in the sense that it can be represented using various series expansions (e.g., expansions in Chebyshev polynomials) the number of terms in which do not depend on the magnitude of  $q$ . In [6], a highly effective numerical method for constructing a nonoscillatory phase function which represents solutions of equations of the form (1) is described.

The scheme of this paper proceeds by first applying the algorithm of [6] in order to obtain a nonoscillatory

phase function  $\alpha$  for (1). We then compute the inverse function  $\alpha^{-1}$  (since  $\alpha$  is an increasing function, it is necessarily invertible). The roots of a solution  $y$  of (1) are calculated using  $\alpha^{-1}$ . In the event that  $y$  is one of the classical orthogonal polynomials, the values of  $y'$  at the roots of  $y$  can also be calculated and used to construct the weights of the corresponding Gaussian quadrature rule. The functions  $\alpha$  and  $\alpha^{-1}$  are represented by piecewise Chebyshev expansions whose number of terms is independent of the magnitude of  $q$ . Both the time required to compute these expansions and the time required to evaluate them is independent of the magnitude of  $q$ . Moreover, once the computation of  $\alpha$  and  $\alpha^{-1}$  is completed, the calculation of each root can be conducted independently. In most circumstances, the cost of computing the phase function  $\alpha$  and its inverse  $\alpha^{-1}$  is small compared to that of calculating all of the roots of the special function on the interval  $[a, b]$ , with the consequence that the algorithm of this paper admits an effective parallel implementation (see, for instance, the experiments presented in Sections 5.3 and 5.5 of this paper).

The remainder of this paper is organized as follows. In Section 1, we briefly review the properties of phase functions. Section 2 discusses nonoscillatory phase functions. In Section 3, we recount the method of [6] for the numerical computation of nonoscillatory phase functions. Section 4 describes the method of this paper for the numerical computation of the roots of special functions satisfying differential equations of the form (1). In Section 5, we describe several numerical experiments conducted to illustrate the properties of the algorithm of Section 4. We conclude with a few remarks in Section 6.

**1. Phase functions and Kummer's equation.** By differentiating (4) twice and adding  $q(t)u(t)$  to both sides of the resulting equation, we see that

$$u''(t) + q(t)u(t) = u(t) \left( q(t) - (\alpha'(t))^2 - \frac{1}{2} \left( \frac{\alpha'''(t)}{\alpha'(t)} \right) + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2 \right) \quad (6)$$

for all  $a < t < b$ . Applying an analogous sequence of steps to (5) shows that

$$v''(t) + q(t)v(t) = v(t) \left( q(t) - (\alpha'(t))^2 - \frac{1}{2} \left( \frac{\alpha'''(t)}{\alpha'(t)} \right) + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2 \right) \quad (7)$$

for all  $a < t < b$ . Since  $\{u, v\}$  is a basis in the space of solutions of (1),  $u$  and  $v$  do not simultaneously vanish. Hence, (6) and (7) imply that  $\alpha$  is a phase function for (1) if and only if its derivative satisfies the second order nonlinear differential equation

$$q(t) - (\alpha'(t))^2 - \frac{1}{2} \left( \frac{\alpha'''(t)}{\alpha'(t)} \right) + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2 = 0 \quad (8)$$

on the interval  $(a, b)$ . We will refer to (8) as Kummer's equation, after Ernst Kummer who studied it in the 1840s [26].

If  $\alpha$  is a phase function for (1), then any solution  $y$  of (1) admits a representation of the form

$$y(t) = c_1 \frac{\cos(\alpha(t))}{\sqrt{\alpha'(t)}} + c_2 \frac{\sin(\alpha(t))}{\sqrt{\alpha'(t)}}. \quad (9)$$

When the coefficient  $q$  is of large magnitude, the magnitude of  $\alpha$  must be large (this is a consequence of the Sturm comparison theorem). In this event, the evaluation of the expression (9) involves the calculation of trigonometric functions of large arguments, and there is an inevitable loss of precision when such calculations are performed in finite precision arithmetic. This is not especially troubling since, except in certain special cases (e.g., Legendre functions of integer orders), a loss of precision in the evaluation of solutions of (1) is inevitable. Indeed, the condition number of the evaluation of a solution  $y$  of (1) is large when  $q$  is large in magnitude.

However, given a phase function  $\alpha$  for (1), the roots

$$t_1, \dots, t_n \quad (10)$$

of a solution  $y$  of (1) and the values

$$y'(t_1), \dots, y'(t_n) \quad (11)$$

of the derivative of  $y$  at the roots (10) can be computed without evaluating trigonometric functions of large arguments and the concomitant loss of precision. To see this, we suppose that  $\alpha$  is a phase function for (1) such that  $\alpha(a) = 0$  and that the values of  $y(a)$  and  $y'(a)$  are known. An elementary calculation shows that

the constants  $c_1$  and  $c_2$  in (9) are given by

$$c_1 = y(a)\sqrt{\alpha'(a)} \quad (12)$$

and

$$c_2 = y(a)\frac{\alpha''(a)}{2(\alpha'(a))^{3/2}} + y'(a)\frac{1}{\sqrt{\alpha'(a)}}. \quad (13)$$

We let  $d_1, d_2$  be the unique pair of real numbers such that  $0 < d_2 \leq \pi$ ,

$$c_1 = d_1 \sin(d_2) \quad (14)$$

and

$$c_2 = d_1 \cos(d_2). \quad (15)$$

Then

$$y(t) = d_1 \frac{\sin(\alpha(t) + d_2)}{\sqrt{\alpha'(t)}} \quad (16)$$

for all  $a \leq t \leq b$ . The expression (16) is highly conducive to computing the roots of  $y$  as well as the values of the derivatives of  $y$  at the roots of  $y$ . Indeed, from (16) it follows that

$$t_j = \alpha^{-1}(j\pi - d_2) \quad (17)$$

for each  $j = 1, 2, \dots, n$ , where  $\alpha^{-1}$  denotes the inverse function of the (monotonically increasing function)  $\alpha$ . By differentiating (16), we obtain

$$y'(t) = d_1 \cos(\alpha(t) + d_2) \sqrt{\alpha'(t)} - d_1 \sin(\alpha(t) + d_2) \frac{\alpha''(t)}{(\alpha'(t))^{3/2}}. \quad (18)$$

Since

$$\sin(\alpha(t_j) + d_2) = \sin(j\pi) = 0 \quad (19)$$

and

$$\cos(\alpha(t_j) + d_2) = \cos(j\pi) = (-1)^j \quad (20)$$

for each  $j = 1, 2, \dots, n$ , we see that

$$y'(t_j) = (-1)^j d_1 \sqrt{\alpha'(t_j)} \quad (21)$$

for each  $j = 1, 2, \dots, n$ . Neither the computation of the constants  $d_1$  and  $d_2$  nor the evaluation of formulas (17), (21) requires the calculation of trigonometric functions of large arguments.

*REMARK 1. An obvious modification of the procedure just described applies in the case where the values of a solution  $y$  of (1) and its derivative are known at arbitrary point in the interval  $[a, b]$ .*

While the condition number of the evaluation of a solution  $y$  of (1) is necessarily large, the condition number of the evaluation of the roots of  $y$  via (17) is equal to the condition number of the phase function  $\alpha$ . Similarly, the time required to calculate a single root of  $y$  using Formula (17) is essentially equal to the cost of evaluating the inverse function  $\alpha^{-1}$ . Analogous remarks apply to Formula (21).

When  $q$  is positive and of large magnitude, almost all phase functions for (1) are highly oscillatory. Indeed, by differentiating the equation

$$\tan(\alpha(t)) = \frac{v(t)}{u(t)}, \quad (22)$$

which is easily obtained from (4) and (5), we see that

$$\alpha'(t) = \frac{W}{(u(t))^2 + (v(t))^2}, \quad (23)$$

where  $W$  is the (necessarily constant) Wronskian of the basis  $\{u, v\}$ . Since  $u$  and  $v$  oscillate rapidly when  $q$  is positive and of large magnitude (this is a consequence of the Sturm comparison theorem), Formula (23) shows that  $\alpha'$ , and hence  $\alpha$ , will oscillate unless some fortuitous cancellation takes place.

When  $\alpha$  oscillates, the the cost and condition number of the evaluation of roots of solutions of (1) via

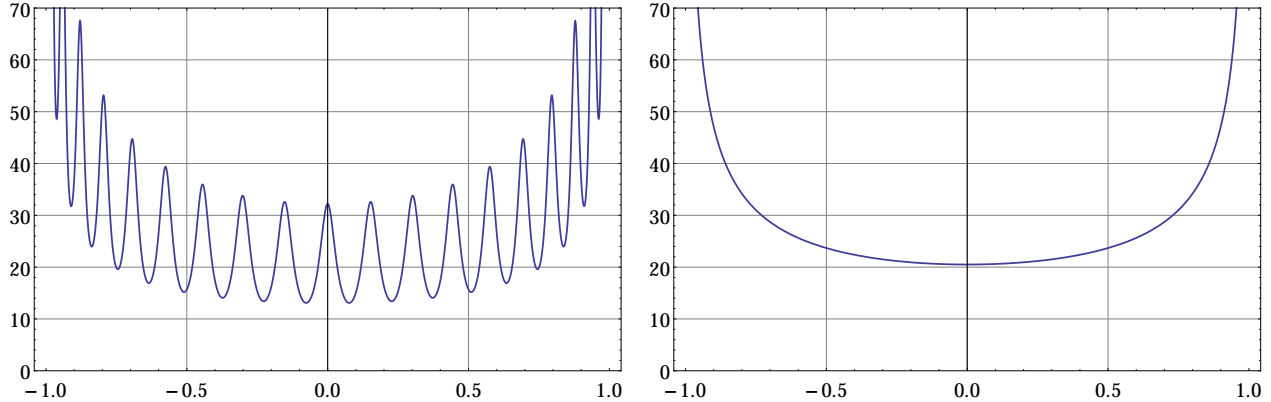


FIG. 1. On the left is a plot of the derivative of a typical (oscillatory) phase function for the normal form (25) of Legendre's differential equation when  $\nu = 20$ . On the right is a plot of the derivative of a nonoscillatory phase function for the same equation when  $\nu = 20$ .

Formula (17) is large. However, the results of [21] and [7], which are the subject of the following section, show that under mild conditions on  $q$  there exists a nonoscillatory phase function for (1). The condition number and cost of the evaluation of nonoscillatory phase functions is small, with the consequence that when such a phase function is available the roots of a solution of (1) can be computed rapidly and to high accuracy via Formula (17). Again, analogous remarks apply to Formula (21).

**2. Nonoscillatory phase functions.** As remarked on earlier, Formula (23) shows that when  $q$  is positive and of large magnitude, the phase function associated with the pair of solutions  $\{u, v\}$  will be oscillatory unless some serendipitous cancellation takes place. In certain cases, a pair  $u, v$  for which this occurs can be obtained by finding a solution of (1) which is an element of one of the Hardy spaces (see, for instance, [13] or [25] for an introduction to the theory of Hardy spaces). Legendre's differential equation

$$(1 - z^2)y''(z) - 2zy'(z) + \nu(\nu + 1)y(z) = 0 \quad (24)$$

provides one such example. It can be transformed into the normal form

$$\psi''(z) + \left( \frac{1}{(1 - z^2)^2} + \frac{\nu(\nu + 1)}{1 - z^2} \right) \psi(z) = 0 \quad (25)$$

by letting

$$\psi(z) = \sqrt{1 - z^2} y(z). \quad (26)$$

According to Formula (9) in Section 3.4 of [11] (see also Formula 8.834.1 in [17]), the function  $f_\nu$  defined for  $x \in \mathbb{R}$  via

$$f_\nu(x) = \left( Q_\nu(x) - i \frac{\pi}{2} P_\nu(x) \right) \sqrt{1 - x^2}, \quad (27)$$

where  $P_\nu$  and  $Q_\nu$  are the Legendre functions of the first and second kinds of degree  $\nu$ , respectively, is the boundary value of the solution

$$F_\nu(z) = (2z)^{-\nu-1} \sqrt{\pi} \frac{\Gamma(\nu + 1)}{\Gamma(\nu + 3/2)} {}_2F_1 \left( \frac{\nu}{2} + 1, \frac{\nu}{2} + \frac{1}{2}; \nu + \frac{3}{2}; \frac{1}{z^2} \right) \sqrt{1 - z^2} \quad (28)$$

of (25). The function  $F_\nu$  is analytic in the upper half-plane and has no zeros there [29]. Moreover, although it is not an element of one of the Hardy spaces on the upper half-plane, its composition with the conformal mapping

$$\tau(z) = i \frac{1 - z}{1 + z} \quad (29)$$

of the unit disk onto the upper half-plane is contained in a Hardy space. The imaginary part of the logarithmic derivative of  $f_\nu$  is, of course, the derivative of a phase function for Legendre's differential equation. That it is nonoscillatory can be established in a number of ways, including via the well-known theorem on the factorization of functions in  $H^p$  spaces (which appears as Theorem 5.5 in [13]). A proof along these lines will

be reported by the author at a later date. Figure 1 depicts this function as well as the derivative of a typical phase function for (25) when  $\nu = 20$ .

This approach can be applied to other equations of interest, including Bessel's equation (see, for instance, [22]), Chebyshev's equation, and the Airy equation. However, it suffers from at least two significant disadvantages: not every differential equation of the form (1) whose coefficient  $q$  is nonoscillatory can be treated in this fashion and, perhaps more seriously, even in cases in which it does apply there is no obvious method for the fast and accurate evaluation of the resulting phase functions.

The first of these difficulties is addressed in [21] and [7]. They contain proofs that, under mild conditions on the coefficient  $q$  appearing in (1), there exists a nonoscillatory function  $\alpha$  such that the functions (4), (5) approximate solutions of (1) with high accuracy. The function  $\alpha$  is nonoscillatory in the sense that it can be represented using various series expansions the number of terms of which does not depend on the magnitude of  $q$ .

We now state a version of the principal result of [7] which pertains to linear ordinary differential equations of the form

$$y''(t) + \lambda^2 q(t)y(t) = 0 \tag{30}$$

with  $\lambda$  a positive real constant and  $q$  a smooth, strictly positive function defined on the real line. The parameter  $\lambda$  is introduced in order to make rigorous the notion of “the magnitude of  $q$ .” The result can be easily applied in cases in which  $q$  varies with  $\lambda$ , as long as  $q$  satisfies the hypotheses of the theorem independent of  $\lambda$ . These requirements are quite innocuous and the theorem can be applied to essentially any ordinary differential equation of the form (1) with  $q$  nonoscillatory. See, for instance, the experiments of Section 5.1 in which  $q$  is taken to be

$$q(t, \lambda) = \lambda^2 \frac{1}{0.1 + t^2} + \lambda^{3/2} \frac{\sin(4t)^2}{(0.1 + (t - 0.5)^2)^4}. \tag{31}$$

See also Figure 2, which contains a plot of the coefficient defined in Formula (31) when  $\lambda = 10^5$  as well as a plot of an associated nonoscillatory phase function.

Similarly, in [7] it is assumed that  $q$  extends to the real line so that the Fourier transform can be used to quantify the notion of “nonoscillatory function.” In most cases of interest, the coefficient  $q$  has either zeros, singularities or both at the endpoints of the interval on which (30) is given. The coefficient  $q$  in (25), for instance, has poles at the points  $\pm 1$ ; nonetheless it can be represented to high relative accuracy via (for instance) polynomials on “graded intervals.” That is,  $q$  can be represented by a polynomial on each subinterval in a collection of subintervals which become smaller as they approach the points  $\pm 1$ . By extending each polynomial to the real line, the results of [7] can be brought to bear on the problem. Note that owing to the assumption that it is analytic,  $q$  can be approximated on a proper subinterval  $[a_0, b_0]$  of  $[a, b]$  to any desired precision  $\epsilon$  via a polynomial  $p$ . Standard results on the continuity of solutions of ordinary differential equations (see, for instance, [9]), imply that by choosing  $\epsilon$  appropriately, the difference in the solutions of (1)

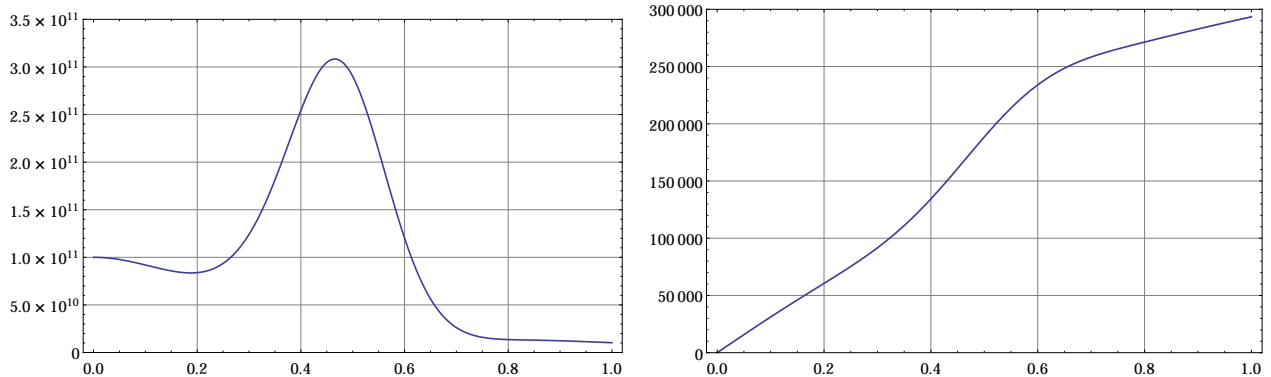


FIG. 2. On the left is a plot of the function (31) when  $\lambda = 10^5$ . On the right is a plot of an associated nonoscillatory phase function.

and those of

$$y''(t) + \lambda^2 p(t)y(t) = 0 \quad (32)$$

can be made arbitrarily small. Equations which have turning points (i.e., locations where the coefficient  $q$  vanishes) at the one or both of the endpoints  $a$  and  $b$  can be dealt with in a similar fashion.

Several definitions are required before stating the principal result of [7]. We say that an infinitely differentiable function  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  is a Schwartz function if

$$\sup_{t \in \mathbb{R}} |t^i \varphi^{(j)}(t)| < \infty \quad (33)$$

for all pairs  $i, j$  of nonnegative integers, and we denote the set of all Schwartz functions by  $S(\mathbb{R})$ . We define functions  $\tilde{p}$  and  $x$  via the formulas

$$\tilde{p}(t) = \frac{1}{q(t)} \left( \frac{5}{4} \left( \frac{q'(t)}{q(t)} \right)^2 - \frac{q''(t)}{q(t)} \right) \quad (34)$$

and

$$x(t) = \int_a^t \sqrt{q(u)} \, du. \quad (35)$$

Since  $q$  is strictly positive,  $x(t)$  is monotonically increasing and hence invertible. We define the function  $p$  via the formula

$$p(x) = \tilde{p}(t(x)); \quad (36)$$

that is,  $p$  is the composition of  $\tilde{p}$  with the inverse function  $t(x)$  of  $x(t)$ . The relationship between the function  $p$  and  $q$  is ostensibly complicated, but, in fact,

$$p(x) = 2 \{t, x\}, \quad (37)$$

where  $\{t, x\}$  denotes the Schwarzian derivative of  $t(x)$ . Note that the Schwarzian derivative  $\{f, x\}$  is defined via the formula

$$\{f, x\} = \frac{f'''(x)}{f'(x)} - \frac{3}{2} \left( \frac{f''(x)}{f'(x)} \right)^2. \quad (38)$$

A derivation of (37) can be found in Section 3 of [7]. The following theorem is a slight reformulation of Theorem 12 in [7].

**THEOREM 1.** *Suppose that the function  $p$  defined via (36) is an element of the Schwartz space  $S(\mathbb{R})$ , that there exist positive real numbers  $\Gamma$  and  $\mu$  such that*

$$|\widehat{p}(\xi)| \leq \Gamma \exp(-\mu|\xi|) \quad \text{for all } \xi \in \mathbb{R}, \quad (39)$$

*and that  $\lambda$  is a positive real number such that*

$$\lambda > 2 \max \left\{ \frac{1}{\mu}, \Gamma \right\}. \quad (40)$$

*Then there exist functions  $\nu$  and  $\delta$  in  $S(\mathbb{R})$  such that*

$$\left| \widehat{\delta}(\xi) \right| \leq \frac{\Gamma}{\lambda^2} \left( 1 + \frac{2\Gamma}{\lambda} \right) \exp(-\mu|\xi|) \quad \text{for all } \xi \in \mathbb{R}, \quad (41)$$

$$\|\nu\|_\infty \leq \frac{\Gamma}{2\mu} \left( 1 + \frac{4\Gamma}{\lambda} \right) \exp(-\mu\lambda), \quad (42)$$

*and the function  $\alpha$  defined via the formula*

$$\alpha(t) = \lambda \sqrt{q(t)} \int_a^t \exp \left( \frac{1}{2} \delta(u) \right) \, du \quad (43)$$

*satisfies the nonlinear differential equation*

$$(\alpha'(t))^2 = \lambda^2 \left( \frac{\nu(t)}{4\lambda^2} + 1 \right) q(t) - \frac{1}{2} \frac{\alpha'''(t)}{\alpha'(t)} + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2. \quad (44)$$



It follows from (44) that  $\alpha$  is a phase function for the perturbed second order linear ordinary differential equation

$$y''(t) + \lambda^2 \left(1 + \frac{\nu(t)}{4\lambda^2}\right) q(t)y(t) = 0, \quad (45)$$

and we conclude from this fact and (42) that when  $\alpha$  is inserted into formulas (4) and (5), the resulting functions approximate solutions of (1) with accuracy on the order of  $\exp(-\mu\lambda)$ . From (41), we conclude that the Fourier transform of  $\delta$  is bounded by  $\exp(-\mu|\xi|)$  for sufficiently large  $\lambda$ . Among other things, this implies that the function  $\delta$  can be represented on the interval  $[a, b]$  on which (1) is given via various series expansions (e.g., as a Chebyshev or Legendre expansion) using a number of terms which does not depend on  $\lambda$ . Plainly, the function  $\alpha$  defined via (43) has this property as well. It is in this sense that  $\alpha$  is nonoscillatory — it can be accurately represented using various series expansions whose number of terms does not depend on the parameter  $\lambda$ . Theorem 1 can be summarized by saying that nonoscillatory phase functions represent the solutions of (30) with  $\mathcal{O}(\exp(-\mu\lambda))$  accuracy using  $\mathcal{O}(1)$  terms. The number of operations required to evaluate Formulas (17) and (21) using the nonoscillatory phase function  $\alpha$  is also independent of  $\lambda$ .

By a slight abuse of terminology, throughout the rest of this article we will refer to the the function  $\alpha$  defined via (43) as the nonoscillatory solution of Kummer's equation and as the nonoscillatory phase function for Equation (30). Note that this function is neither an exact solution of (8) (although it approximates a solution of that equations with error which decays exponentially with  $\lambda$ ), nor is it unique (but there is one and only one nonoscillatory phase function associated with Theorem 1).

**3. A practical method for the computation of nonoscillatory phase functions.** The method used in [21] and [7] to prove the existence of nonoscillatory phase function is constructive and could serve as the basis of a numerical algorithm for their computation. However, such an approach would require that  $q$  be explicitly extended to the real line as well as knowledge of the first two derivatives of  $q$ . We now describe a minor variant of the algorithm of [6]. Under the hypotheses of Theorem 1, it results in a nonoscillatory function  $\alpha$  which represents solutions of (30) with accuracy on the order of  $\exp(-\frac{1}{2}\mu\lambda)$ , where  $\mu$  is the constant appearing in Theorem 1. The method of [6] has the advantage that it only requires knowledge of the coefficient  $q$  on the interval  $[a, b]$ . Note that, as is the case with Theorem 1, there is no difficulty in treating equations in which the coefficient  $q$  varies with  $\lambda$ .

The algorithm proceeds as follows. First, a windowed version  $\tilde{q}$  of  $q$  which closely agrees with  $q$  on the rightmost quarter of the interval  $[a, b]$  and is approximately equal to the constant 1 on the leftmost quarter of  $[a, b]$  is constructed. More specifically,  $\tilde{q}$  is defined via the formula

$$\tilde{q}(t) = \phi(t) + (1 - \phi(t))q(t), \quad (46)$$

where  $\phi$  is given by

$$\phi(t) = \frac{1}{2} \left( \operatorname{erf} \left( \frac{24}{b-a} \left( t + \frac{a+b}{2} \right) \right) - \operatorname{erf} \left( \frac{24}{b-a} \left( t - \frac{a+b}{2} \right) \right) \right). \quad (47)$$

We use the analytic windowing function  $\phi$  to construct  $\tilde{q}$  (as opposed to a windowing function which is infinitely differentiable and compactly supported) so that we can apply Theorem 1 to the windowed version  $\tilde{q}$  of  $q$  (its hypotheses imply that  $q$  is analytic in a strip containing the real line). The constants in (47) are set so that

$$1 - \phi(t) < 10^{-16} \quad \text{for all } t \leq \frac{3a+b}{4} \quad (48)$$

and

$$\phi(t) < 10^{-16} \quad \text{for all } t \geq \frac{a+3b}{4}. \quad (49)$$

Figure 3 shows the function  $\phi$  when  $a = 0$  and  $b = 1$ ; it also contains plots of  $q$  and  $\tilde{q}$  when the coefficient is taken to be  $q(t) = t/(0.5 + t^2)^2$ . Next, a solution  $\tilde{\alpha}'$  of the initial value problem

$$\begin{cases} \lambda^2 \tilde{q}(t) - (\tilde{\alpha}'(t))^2 - \frac{1}{2} \frac{\tilde{\alpha}'''(t)}{\tilde{\alpha}'(t)} + \frac{3}{4} \left( \frac{\tilde{\alpha}''(t)}{\tilde{\alpha}'(t)} \right)^2 = 0 & \text{for all } a \leq t \leq b \\ \tilde{\alpha}'(a) = \lambda \\ \tilde{\alpha}''(a) = 0 \end{cases} \quad (50)$$



is obtained. A plot of the solution of the boundary value problem (50) when  $q(t) = t/(0.5 + t^2)^2$  and  $\lambda = 10^5$  is shown in the lower right hand corner of Figure 3. The initial conditions  $\tilde{\alpha}'(a) = \lambda$  and  $\tilde{\alpha}''(a) = 0$  in (50) are chosen because the nonoscillatory phase function for the equation

$$y''(t) + \lambda^2 \tilde{q}(t)y(t) = 0 \quad (51)$$

whose existence is ensured by Theorem 1 behaves as

$$\lambda t + O\left(\exp\left(-\frac{1}{2}\mu\lambda\right)\right) \quad (52)$$

on the leftmost quarter of the interval  $[a, b]$  where  $\lambda^2 \tilde{q}$  is approximately equal to the constant  $\lambda^2$ . This

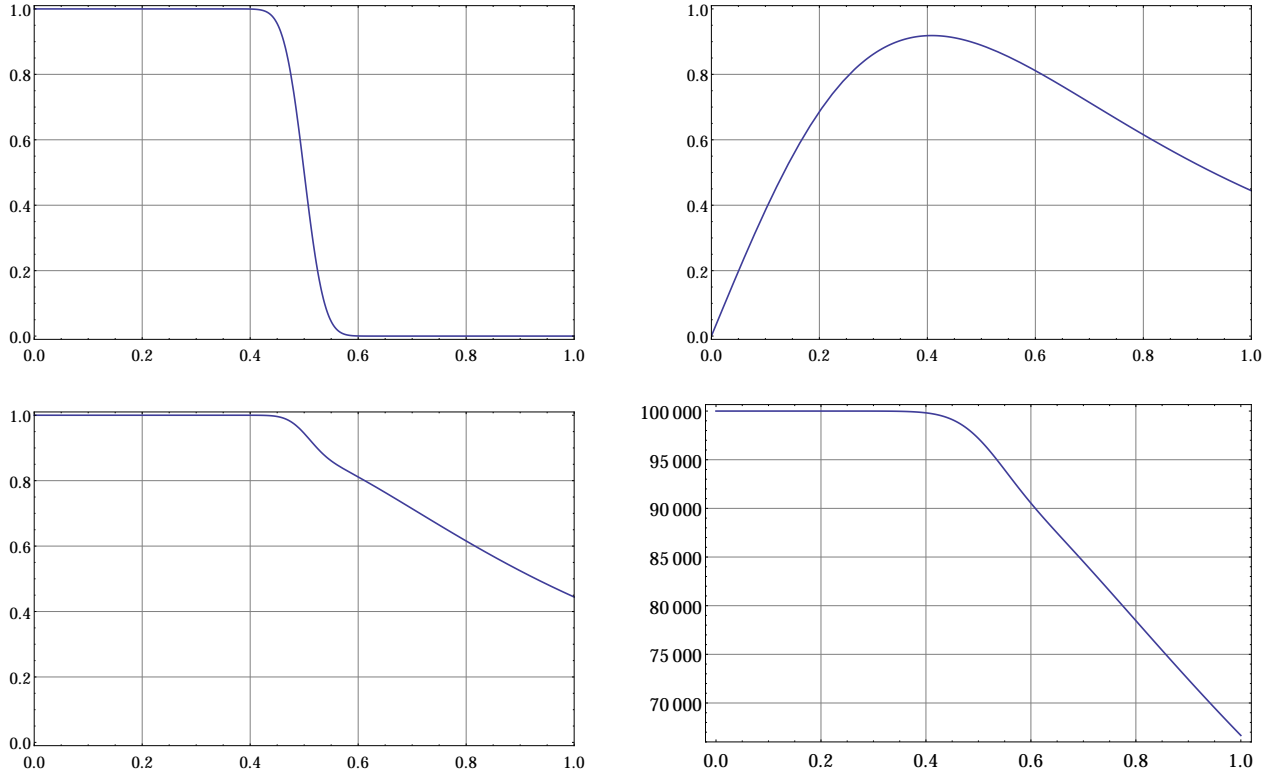


FIG. 3. At the top left is a plot of the function  $\phi$  defined by (47) when  $a = 0$  and  $b = 1$ . A plot of the coefficient  $q(t) = t/(t+0.5)^2$  appears at the top right. At the bottom left is the windowed version of  $q$ , defined via (46). It closely agrees with  $q$  on the rightmost quarter of the interval  $[0, 1]$  and is nearly constant on the leftmost quarter of  $[0, 1]$ . At the bottom right is the derivative of the nonoscillatory phase function  $\tilde{\alpha}$  obtained by solving (53) with  $\lambda = 10^5$ .

estimate is proven in [6]. It is also shown in [6] that on the rightmost quarter of the interval  $[a, b]$  the difference between the nonoscillatory phase function for Equation (30) and the solution  $\tilde{\alpha}$  of (50) is on the order of  $\exp(-\frac{1}{2}\mu\lambda)$  as is the difference between  $\tilde{\alpha}'$  and the derivative of the nonoscillatory phase function for Equation (30). It follows that by solving the initial value problem (50) we approximate the values of the nonoscillatory phase function for (30) and its derivative at the right-hand endpoint  $b$  with accuracy on the order of  $\exp(-\frac{1}{2}\mu\lambda)$ . The algorithm concludes by solving the terminal value problem

$$\begin{cases} \lambda^2 q(t) - (\alpha'(t))^2 - \frac{1}{2} \frac{\alpha'''(t)}{\alpha'(t)} + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2 = 0 & \text{for all } a \leq t \leq b \\ \alpha'(b) = \tilde{\alpha}'(b) \\ \alpha''(b) = \tilde{\alpha}''(b). \end{cases} \quad (53)$$

Standard results on the continuity of solutions of ordinary differential equations (see, for instance, [9]) together with the preceding estimate imply that the solution  $\alpha$  of (53) approximates the nonoscillatory phase function for Equation (30) on the interval  $[a, b]$  with accuracy on the order of  $\exp(-\frac{1}{2}\mu\lambda)$ .

**4. An algorithm for the computation of the roots of special functions.** In this section, we describe an algorithm for computing the roots

$$t_1 < t_2 < \dots < t_n \quad (54)$$

on the interval  $[a, b]$  of a solution  $y$  of Equation (30), as well as the values of the derivative of  $y$  at the points (54). It takes as inputs the value of  $\lambda$ , a subroutine for evaluating the coefficient  $q$  in (1), the values of the function  $y$  and its derivative at the left-hand end point  $a$  of the interval  $[a, b]$  on which (1) is given, a positive integer  $k$ , and a partition

$$a = \gamma_1 < \gamma_2 < \dots < \gamma_m < \gamma_{m+1} = b \quad (55)$$

of the interval  $[a, b]$ . As with the analyses of Sections 2 and 3, the algorithm described here can be easily adapted to the case in which the coefficient  $q$  varies with  $\lambda$ .

The algorithm proceeds as follows:

1. We construct a nonoscillatory solution  $\tilde{\alpha}$  of the initial value problem (50). Then, having obtained the values of  $\tilde{\alpha}(a)$  and  $\tilde{\alpha}(b)$ , we solve the terminal value problem (53). The resulting function  $\alpha$  is a nonoscillatory solution of Kummer's equation.
2. We next construct the inverse function  $\alpha^{-1}$  of the monotonically increasing function  $\alpha$  on the interval  $[\alpha(a), \alpha(b)]$  via Newton's method.
3. Then, we calculate the coefficients  $c_1$  and  $c_2$  such that

$$y(t) = c_1 \frac{\cos(\alpha(t))}{\sqrt{\alpha'(t)}} + c_2 \frac{\sin(\alpha(t))}{\sqrt{\alpha'(t)}} \quad (56)$$

using Formulas (12) and (13). We determine  $d_1$  and  $d_2$  such that

$$y(t) = d_1 \frac{\sin(\alpha(t) + d_2)}{\sqrt{\alpha'(t)}} \quad (57)$$

using the relations (14), (15).

4. Finally, we use Formula (17) to calculate the  $j^{\text{th}}$  root  $t_j$  of  $y$  on the interval  $[a, b]$  and (21) to calculate the value of  $y'$  at  $t_j$

Of course, once Steps 1-4 have been completed, the roots  $t_j$  and corresponding values  $y'(t_j)$  can be computed in any order using Formulas (17) and (21).

The function  $\alpha$  is represented by its values at the  $k$ -point Chebyshev grids on each of the  $m$  subintervals

$$[\gamma_1, \gamma_2], [\gamma_2, \gamma_3], \dots, [\gamma_m, \gamma_{m+1}]. \quad (58)$$

The  $k$ -point Chebyshev grid on  $[\gamma_i, \gamma_{i+1}]$  is the set

$$\left\{ \frac{\gamma_{i+1} + \gamma_i}{2} + \frac{\gamma_{i+1} - \gamma_i}{2} \cdot \cos\left(\frac{l\pi}{k-1}\right) : l = 0, 1, \dots, k-1 \right\}. \quad (59)$$

Given the values of a polynomial of degree  $k-1$  at the points (59), its value at any point on the interval  $[\gamma_i, \gamma_{i+1}]$  can be calculated in a numerically stable fashion in  $\mathcal{O}(k)$  operations via barycentric interpolation. Moreover, assuming the partition (55) is properly chosen, barycentric interpolation can be used to approximate value of  $\alpha$  at any point  $x$  in  $[a, b]$  given its values at the Chebyshev nodes on the subintervals (58). This can be done in  $\mathcal{O}(k + \log_2(m))$  operations by first finding the subinterval containing  $x$  using a binary search and then performing barycentric interpolation on that subinterval. See, for instance, [35] for an extensive discussion of Chebyshev polynomials and interpolation. In the experiments described in Section 5 of this paper,  $k$  took on various values between 5 and 30.

The problems (50) and (53) are stiff when  $\lambda$  is large and an appropriately chosen method must be used to solve them numerically. We compute the values of the solutions at the  $k$ -point Chebyshev grid on each of the subintervals  $[\gamma_i, \gamma_{i+1}]$  by first constructing a low-accuracy approximation to the solution via the implicit trapezoidal method (see, for instance, [23]), and then applying the Newton-Kantorovich method (which is discussed in Chapter 5 of [37], among many other sources). We now describe the specifics of the Newton-Kantorovich method in more detail. By multiplying both sides of Kummer's equation

$$\lambda^2 q(t) - (\alpha'(t))^2 - \frac{1}{2} \frac{\alpha'''(t)}{\alpha'(t)} + \frac{3}{4} \left( \frac{\alpha''(t)}{\alpha'(t)} \right)^2 = 0 \quad (60)$$

by  $\alpha'$ , letting  $\beta(t) = \alpha'(t)$  and rearranging the terms of the resulting equation, we arrive at the differential

equation

$$\beta''(t) + 2(\beta(t))^3 - 2\lambda^2 q(t)\beta(t) - \frac{3}{2} \frac{\beta'(t)}{\beta(t)} = 0. \quad (61)$$

In each iteration of Newton-Kantorovich method, a given approximation  $\beta_0$  of the solution of (61) is updated by solving the linearized equation

$$\delta''(t) + \left( 3 \frac{\beta_0'(t)}{\beta_0(t)} \right) \delta'(t) + \left( 6(\beta_0(t))^2 + \frac{3}{2} \frac{(\beta_0'(t))^2}{(\beta_0(t))^2} - 2\lambda^2 q(t) \right) \delta(t) = r(t), \quad (62)$$

where

$$r(t) = -\beta_0''(t) - 2(\beta_0(t))^3 + 2\lambda^2 q(t)\beta_0(t) + \frac{3}{2} \frac{\beta_0'(t)}{\beta_0(t)}, \quad (63)$$

for  $\delta$  and taking the new approximation of the solution of (61) to be  $\beta_0 + \delta$ . The second order linear differential equation (62) is solved via a variant of the spectral method of [18]. Newton-Kantorovich iterations are continued until no further improvement in the solution  $\beta$  is obtained. A solution  $\alpha$  of Kummer's equation (60) such that  $\alpha(a) = 0$  is obtained from  $\beta$  through the formula

$$\alpha(t) = \int_a^t \beta(u) du. \quad (64)$$

The inverse phase function  $\alpha^{-1}$  is represented via its values on the  $k$ -point Chebyshev grids on each of the  $m$  subintervals

$$[\alpha(\gamma_1), \alpha(\gamma_2)], [\alpha(\gamma_2), \alpha(\gamma_3)], \dots, [\alpha(\gamma_m), \alpha(\gamma_{m+1})]. \quad (65)$$

There are  $m(k-1) + 1$  such points (since the set (59) includes the endpoints of each interval), and we denote them by

$$\rho_1 < \rho_2 < \dots < \rho_{m(k-1)+1}. \quad (66)$$

The values of  $\alpha^{-1}$  at the endpoints of the intervals (65) are (obviously) known. We calculate its values at the remaining points via Newton's method. Since  $\alpha$  is monotonically increasing, we start the process by evaluating  $\alpha^{-1}$  at  $\rho_{m(k-1)}$ , then at  $\rho_{m(k-1)-1}$ , and so on. As in the case of  $\alpha$ , once the values of  $\alpha^{-1}$  at the points (66) are known, the value of  $\alpha^{-1}$  at any point on the interval  $[\alpha(a), \alpha(b)]$  can be approximated in  $\mathcal{O}(k + \log_2(m))$  operations via barycentric interpolation.

In some cases, an appropriate collection of subintervals (58) is not known *a priori* and must be determined through an adaptive procedure. In that event, we construct an initial set of subintervals by adaptively discretizing the function  $\sqrt{q(t)}$ . We use  $\sqrt{q(t)}$  as a starting point for the representation of  $\alpha'$  because of the classical estimate

$$\alpha'(t) = \lambda\sqrt{q(t)} + O(1); \quad (67)$$

see, for instance, [12]. We note too that when inserted into (4) and (5), the crude approximation

$$\alpha(t) \approx \lambda \int_a^t \sqrt{q(u)} du \quad (68)$$

gives rise to the first order WKB approximations of the solutions of (30). The adaptive discretization of  $\sqrt{q(t)}$  proceeds by recursively subdividing the interval  $[a, b]$  until each of the resulting subintervals  $[a_0, b_0]$  satisfy the following property. Suppose that

$$\sum_{l=0}^{k-1} c_l T_l(t) \quad (69)$$

is the Chebyshev expansion of the polynomial of degree  $k-1$  which interpolates  $\sqrt{q(t)}$  at the nodes of the  $k$ -point Chebyshev grid on the subinterval  $[a_0, b_0]$ , and that

$$c_{\max} = \max\{|c_0|, |c_1|, \dots, |c_{k-1}|\}. \quad (70)$$

We subdivide  $[a_0, b_0]$  if any of the quantities

$$\frac{|c_{\lceil k/2 \rceil}|}{c_{\max}}, \dots, \frac{|c_{k-1}|}{c_{\max}} \quad (71)$$

are greater than a specified value (which was taken to be  $10^{-13}$  in the experiments described in Section 5 of this paper).

The collection of subintervals obtained by discretizing  $\sqrt{q(t)}$  might not suffice for representing the solution  $\alpha$  of Kummer’s equation. Accordingly, we follow the following procedure while solving the problems (50) and (53). After using the Newton-Kantorovich method as described above to approximate the values of the solution  $f$  of one of these problems on a subinterval  $[a_0, b_0]$ , we compute the coefficients  $c_0, c_1, \dots, c_{k-1}$  in the expansion (69) of the polynomial of degree  $k - 1$  interpolating  $f$  at the nodes of the  $k$ -point Chebyshev grid on  $[a_0, b_0]$ . We apply the same criterion as before in order to decide whether to divide the interval  $[a_0, b_0]$  or not; that is, if the relative magnitude of one the trailing coefficients in that expansion is too large, then the interval  $[a_0, b_0]$  is split in half and the same procedure is applied, recursively, to each of the two resulting subintervals of  $[a_0, b_0]$ .

REMARK 2. *It is possible that the collection of subintervals (65) is insufficient to represent the function  $\alpha^{-1}$ ; however, we have never seen this occur in practice. Indeed, an early version of the algorithm of this paper adaptively discretized  $\alpha^{-1}$  independently of  $\alpha$ , but this code was removed as it was never necessary. Similarly, we have never encountered any numerical difficulties in using Newton’s method to compute the inverse function  $\alpha^{-1}$  to high precision.*

REMARK 3. *The procedure for the numerical solution of the boundary value problems (50) and (53) described here was chosen for its robustness and its ability to solve extremely stiff ordinary differential equations to high accuracy. In the numerical experiments of Section 5.3, for instance, values of  $\lambda$  as large as  $10^{12}$  are considered. When the value of  $\lambda$  is somewhat smaller, faster methods — such as the spectral deferred correction method of [10] — may be used in place of the technique described here.*

**5. Numerical experiments.** In this section, we describe several numerical experiments which were conducted to illustrate the performance of the algorithm of this article. Our code was written in Fortran 95 using OpenMP extensions and compiled with the Intel Fortran Compiler version 16.0.0. All calculations were carried out on a desktop computer equipped with 28 Intel Xeon E5-2697 processor cores running at 2.6 GHz and 512 GB of memory. A version of the code used to conduct these experiments is available at the author’s website: <http://www.math.ucdavis.edu/~bremer/code.html>.

**5.1. An artificial example.** For various values of  $\lambda$ , we computed the roots of the solution of the initial value problem

$$\begin{cases} y''(t) + q(t, \lambda)y(t) = 0 & \text{for all } 0 \leq t \leq 1 \\ y(0) = 0 \\ y'(0) = \lambda, \end{cases} \quad (72)$$

TABLE 1

*The results of the experiment of Section 5.1. These calculations were performed using a single processor core. All times are in seconds.*

$\lambda$	Phase function time	Number of roots in $[0, 1]$	Root calculation time
$10^3$	$7.03 \times 10^{-02}$	2096	$2.66 \times 10^{-04}$
$10^4$	$3.49 \times 10^{-02}$	13,339	$2.05 \times 10^{-03}$
$10^5$	$3.18 \times 10^{-02}$	93,398	$1.47 \times 10^{-02}$
$10^6$	$2.88 \times 10^{-02}$	736,207	$9.78 \times 10^{-02}$
$10^7$	$2.61 \times 10^{-02}$	6,476,851	$7.07 \times 10^{-01}$
$10^8$	$3.00 \times 10^{-02}$	61,289,533	$5.02 \times 10^{+00}$
$10^9$	$3.59 \times 10^{-02}$	600,685,068	$4.63 \times 10^{+01}$

where  $q$  is defined via the formula

$$q(t, \lambda) = \lambda^2 \frac{1}{0.1 + t^2} + \lambda^{3/2} \frac{\sin(4t)^2}{(0.1 + (t - 0.5)^2)^4}. \quad (73)$$

The adaptive version of the algorithm of Section 4 was used and the parameter  $k$  was taken to be 16. Table 1 presents the results. There, each row corresponds to one value of  $\lambda$  and reports the time (in seconds) required to construct the nonoscillatory phase function and its inverse, the number of roots of the solution of (72) in the interval  $[0, 1]$ , and the time required to compute the roots. Figure 2 displays the coefficient (73) when  $\lambda = 10^5$ , as well as a plot of an associated nonoscillatory phase function. Figure 4 shows the inverse of that nonoscillatory phase function.

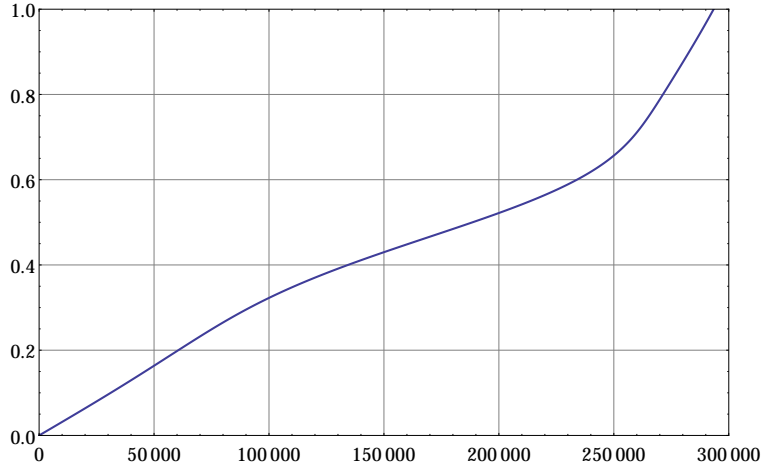


FIG. 4. The inverse function of the nonoscillatory phase function depicted in Figure 2.

**5.2. Gauss-Legendre quadrature formulas.** The Legendre polynomial  $P_n$  of degree  $n$  is a solution of the ordinary differential equation

$$(1 - t^2)\varphi''(t) - 2t\varphi'(t) + n(n + 1)\varphi(t) = 0 \quad \text{for all } -1 \leq t \leq 1. \quad (74)$$

Its roots

$$-1 < t_1 < t_2 < \dots < t_n < 1 \quad (75)$$

are the nodes of the  $n$ -point Gauss-Legendre quadrature rule, and the corresponding weights  $w_1, \dots, w_n$  are given by

$$w_j = \frac{2}{(P'_n(t_j))^2 (1 - t_j^2)}. \quad (76)$$

Formula (76) can be found in many references; it is a special case of of Formula 15.3.1 in [33], for instance. Since the Legendre polynomial  $P_n$  satisfies the symmetry relation

$$P_n(-t) = (-1)^n P_n(t), \quad (77)$$

it suffices to compute its roots on the interval  $[0, 1]$ . Rather than computing the roots of the function  $P_n$  on  $[0, 1]$ , we calculated the roots of the function

$$z_n(\theta) = P_n(\cos(\theta))\sqrt{\sin(\theta)}, \quad (78)$$

which is a solution of the second order differential equation

$$z''(\theta) + \left( \frac{1}{2} + n + n^2 + \frac{1}{4} \cot(\theta)^2 \right) z(\theta) = 0 \quad (79)$$

on the interval  $(0, \pi/2]$ . That (78) satisfies (79) can be verified directly by plugging (78) into (79) and making use of the fact that  $P_n$  satisfies (74). The introduction of the new dependent variable  $\theta = \arccos(t)$  in (74) is suggested in [32] as a way to mitigate the numerical problems caused by the clustering of Gauss-Legendre quadrature nodes near the points  $\pm 1$ , and the presence of the factor  $\sqrt{\sin(\theta)}$  ensures that the transformed

equation is of the form (1). See [32] and [4] for discussions of the numerical issues which arise from the clustering of Gauss-Legendre nodes near  $\pm 1$ .

The coefficient in (79) is singular at the origin; consequently, we represented  $\alpha$  and  $r$  using a “graded mesh” of points which cluster near 0. More specifically, the functions  $\alpha$  and  $r$  were represented via their values at the 5-point Chebyshev grids on the 3473 intervals

$$[\gamma_1, \gamma_2], [\gamma_2, \gamma_3], \dots, [\gamma_{3473}, \gamma_{3474}], \quad (80)$$

where

$$\gamma_i = \frac{\pi}{2} \cdot (1.01)^{-3474+i}. \quad (81)$$

Low order expansions were used in order to ensure that the functions  $\alpha$  and  $\alpha'$  could be evaluated quickly. When higher order expansions are used, the resulting phase functions can be stored much more efficiently (see, for instance, the experiments of Section 5.3).

The coefficients  $c_1$  and  $c_2$  such that

$$z_n(\theta) = c_1 \frac{\cos(\alpha(\theta))}{\sqrt{\alpha'(\theta)}} + c_2 \frac{\sin(\alpha(\theta))}{\sqrt{\alpha'(\theta)}} \quad (82)$$

were obtained via Formulas (12) and (13); the values of  $z_n$  and its derivative  $z'_n$  at the point

$$\gamma_1 = \pi/2(1.01)^{-3473} \approx 1.54166044582463 \times 10^{-15}, \quad (83)$$

which are needed in (12) and (13), were approximated using the expansion

$$P_n(\cos(\theta))\sqrt{\sin(\theta)} \approx \sqrt{\theta} + \theta^{5/2} \left( -\frac{n^2}{4} - \frac{n}{4} - \frac{1}{12} \right) + \theta^{9/2} \left( \frac{n^4}{64} + \frac{n^3}{32} + \frac{5n^2}{192} + \frac{n}{96} + \frac{1}{1440} \right) + \mathcal{O}(\theta^{13/2}n^6). \quad (84)$$

The expansion (84) can be easily derived from Formula 8.702 in [17]. The real numbers  $d_1$  and  $d_2$  such that

$$z_n(\theta) = d_1 \frac{\sin(\alpha(\theta) + d_2)}{\sqrt{\alpha'(\theta)}} \quad (85)$$

were computed from  $c_1$  and  $c_2$  using (14) and (15). The roots (75) of  $P_n$  are related to the roots  $\theta_1 < \theta_2 < \dots < \theta_{\lceil n/2 \rceil}$  of  $z_n$  via the formula

$$t_j = \begin{cases} -\cos(\theta_j) & \text{if } 1 \leq j \leq \lceil \frac{n}{2} \rceil \\ \cos(\theta_{n-j+1}) & \text{if } \lceil \frac{n}{2} \rceil < j \leq n. \end{cases} \quad (86)$$

TABLE 2

*A comparison of the time taken to construct Gauss-Legendre quadrature rules of various orders using the approach of this paper and the specialized approach of [3]. These computations were performed using a single processor core. All times are in seconds.*

Order (n)	Phase function time	Quadrature evaluation time	Total running time	Running time of the algorithm of [3]	Maximum relative difference in weights
10 <sup>3</sup>	8.70×10 <sup>-02</sup>	3.74×10 <sup>-04</sup>	8.74×10 <sup>-02</sup>	1.49×10 <sup>-04</sup>	2.31×10 <sup>-14</sup>
10 <sup>4</sup>	9.28×10 <sup>-02</sup>	2.52×10 <sup>-03</sup>	9.54×10 <sup>-02</sup>	2.20×10 <sup>-03</sup>	3.34×10 <sup>-14</sup>
10 <sup>5</sup>	4.45×10 <sup>-02</sup>	7.37×10 <sup>-03</sup>	5.18×10 <sup>-02</sup>	8.43×10 <sup>-03</sup>	5.88×10 <sup>-14</sup>
10 <sup>6</sup>	4.66×10 <sup>-02</sup>	7.67×10 <sup>-02</sup>	1.23×10 <sup>-01</sup>	8.64×10 <sup>-02</sup>	1.31×10 <sup>-14</sup>
10 <sup>7</sup>	4.62×10 <sup>-02</sup>	7.21×10 <sup>-01</sup>	7.67×10 <sup>-01</sup>	7.93×10 <sup>-01</sup>	1.21×10 <sup>-14</sup>
10 <sup>8</sup>	4.31×10 <sup>-02</sup>	7.22×10 <sup>+00</sup>	7.32×10 <sup>+00</sup>	8.13×10 <sup>+00</sup>	1.26×10 <sup>-14</sup>
10 <sup>9</sup>	4.79×10 <sup>-02</sup>	7.02×10 <sup>+01</sup>	7.02×10 <sup>+01</sup>	7.91×10 <sup>+01</sup>	1.32×10 <sup>-14</sup>
10 <sup>10</sup>	4.87×10 <sup>-02</sup>	7.23×10 <sup>+02</sup>	7.23×10 <sup>+02</sup>	8.20×10 <sup>+02</sup>	1.41×10 <sup>-14</sup>

Moreover, if  $t_j = \pm \cos(\theta)$ , then

$$\frac{z'_n(\theta)}{\sqrt{\sin(\theta)}} = -P'_n(\cos(\theta)) \sin(\theta)^2 = P'_n(t_j) \sqrt{1 - t_j^2}. \quad (87)$$

By combining (21), (76), (86) and (87), we obtain the formula

$$w_j = \begin{cases} \frac{2 \sin(\theta_j)}{d_1^2 \alpha'(\theta_j)} & \text{if } 1 \leq j \leq \left\lceil \frac{n}{2} \right\rceil \\ \frac{2 \sin(\theta_{n-j+1})}{d_1^2 \alpha'(\theta_{n-j+1})} & \text{if } \left\lceil \frac{n}{2} \right\rceil < j \leq n, \end{cases} \quad (88)$$

which expresses the  $j^{\text{th}}$  Gauss-Legendre weight in terms of the derivative of the phase function  $\alpha$ .

For several values of  $n$ , we compared the time taken to compute the nodes and weights of the  $n$ -point Gauss-Legendre quadrature via by the algorithm of this paper with the time required to do so via the algorithm of [3]. We used the C++ implementation [2] made available by the author of [3]. These calculations were performed using a single processor core. Table 2 reports the results as well as the largest relative difference in the weights for each value of  $n$ . We observe that (surprisingly, given its great generality) the algorithm of this paper is competitive with that of [3] when  $n$  is sufficiently large.

**5.3. Gauss-Jacobi quadrature formulas.** The Jacobi polynomial  $P_n^{(\gamma, \zeta)}$  is a solution of the second order linear ordinary differential equation

$$(1 - t^2)\varphi''(t) + (\zeta - \gamma - (\gamma + \zeta + 2)t)\varphi'(t) + n(n + \gamma + \zeta + 1)\varphi(t) = 0. \quad (89)$$

Its roots

$$-1 < t_1 < t_2 < \dots < t_n < 1 \quad (90)$$

are the nodes of the Gauss-Jacobi quadrature rule

$$\int_{-1}^1 f(t)(1-t)^\gamma(1+t)^\zeta dt \approx \sum_{j=1}^n f(t_j)w_j, \quad (91)$$

which is exact for polynomials of degree  $2n - 1$ . The weights  $w_1, \dots, w_n$  are given by the formula

$$w_j = \frac{\Gamma(n + \gamma + 1)\Gamma(n + \zeta + 1)}{\Gamma(n + 1)\Gamma(n + \gamma + \zeta + 1)} \frac{2^{\gamma + \zeta + 1}}{(1 - t_j^2) \left( P_n^{(\gamma, \zeta)'}(t_j) \right)^2}. \quad (92)$$

See, for instance, Section 15.3 in [33] for more information regarding Gauss-Jacobi quadratures, including a derivation of Formula (92).

As in the special case of Gauss-Legendre quadrature rules, we introduce a change of variables in order to avoid the problems associated with the clustering of the nodes (90) near  $\pm 1$ ; see [20] for further discussion of this phenomenon. If  $Q_n^{(\gamma, \zeta)}$  and  $r^{(\gamma, \zeta)}$  are the functions defined via

$$r^{(\gamma, \zeta)}(\theta) = \left( \cot\left(\frac{\theta}{2}\right) \right)^{\frac{\zeta - \gamma}{2}} \left( \sin\left(\frac{\theta}{2}\right) \right)^{\frac{1 + \gamma + \zeta}{2}} (\sin(\theta))^{\frac{\gamma + \zeta + 1}{2}} \quad (93)$$

and

$$Q_n^{(\gamma, \zeta)}(\theta) = n(\gamma + \zeta + n + 1) - \frac{1}{4} \csc^2(t)(\gamma - \zeta + (\gamma + \zeta + 1) \cos(t))^2 + \frac{1}{2} \csc^2(t)(\gamma + \zeta + (\gamma - \zeta) \cos(t) + 1), \quad (94)$$

then the function  $z_n^{(\gamma, \zeta)}$  defined by

$$z_n^{(\gamma, \zeta)}(\theta) = P_n^{(\gamma, \zeta)}(\cos(\theta))r^{(\gamma, \zeta)}(\theta) \quad (95)$$

satisfies the second order equation

$$y''(\theta) + Q_n^{(\gamma, \zeta)}(\theta)y(\theta) = 0 \quad (96)$$

on the interval  $(0, \pi/2]$ .

The behavior of the coefficient in (96) depends strongly on  $\gamma$  and  $\zeta$  — indeed, it is singular in some cases and smooth on the whole interval  $[0, \pi/2]$  in others. Accordingly, for various values of  $\gamma$  and  $\zeta$ , we



used the adaptive version of the algorithm of Section 4 in order to construct a nonoscillatory phase function  $\alpha^{(\gamma,\zeta)}$  representing  $z_n^{(\gamma,\zeta)}$  on the interval  $(10^{-15}, 1)$ . Table 3 reports the size of the piecewise Chebyshev expansions used to represent the nonoscillatory phase function in each case. More specifically, the associated nonoscillatory phase functions were represented via their values at the nodes of the 30 point Chebyshev grids on a collection of subintervals and Table 3 lists the number of subintervals in each case and the total number of values used to represent each of the nonoscillatory phase functions. We refer to this last quantity, which is equal to  $29m + 1$ , where  $m$  is the number of subintervals into which  $[0, \pi/2]$  is divided, as the “expansion size” for want of a better term.

The values of  $z_n^{(\gamma,\zeta)}$  and its derivative at the point  $1.0 \times 10^{-15}$ , which are needed to calculate the constants  $d_1^{(\gamma,\zeta)}$  and  $d_2^{(\gamma,\zeta)}$  such that

$$z_n^{(\gamma,\zeta)}(\theta) = d_1^{(\gamma,\zeta)} \frac{\sin\left(\alpha^{(\gamma,\zeta)}(t) + d_2^{(\gamma,\zeta)}\right)}{\sqrt{\alpha^{(\gamma,\zeta)'}(t)}}, \quad (97)$$

were computed using a 7-term Taylor expansion for  $z_n^{(\gamma,\zeta)}$  around the point 0. This expression is too cumbersome to reproduce here, but it can be derived easily starting from the well-known representation of  $P_n^{(\gamma,\zeta)}$  in terms of Gauss’ hypergeometric function (see, for instance, Formula (4.21.2) in [33]).

Since

$$P_n^{(\gamma,\zeta)}(t) = (-1)^n P_n^{(\zeta,\gamma)}(t), \quad (98)$$

the roots of  $P_n^{(\gamma,\zeta)}$  in the interval  $[-1, 1]$  can be obtained by computing the roots of  $z_n^{(\gamma,\zeta)}$  in the interval

TABLE 3

*The size of the piecewise Chebyshev expansions used to represent the nonoscillatory phase function representing the solution of  $z_n^{(\gamma,\zeta)}$  of Equation (96). The zeros of  $z_n^{(\gamma,\zeta)}$  on the interval  $[0, \pi/2]$  are related to those of the Jacobi polynomial  $P_n^{(\gamma,\zeta)}$  on the interval  $[0, 1]$  through Formula (101).*

$\gamma$	$\zeta$	n	Number of subintervals	Expansion size	$\gamma$	$\zeta$	n	Number of subintervals	Expansion size
-0.30	0.25	10 <sup>3</sup>	97	2814	0.25	-0.30	10 <sup>3</sup>	97	2814
		10 <sup>4</sup>	92	2669			10 <sup>4</sup>	92	2669
		10 <sup>5</sup>	89	2582			10 <sup>5</sup>	89	2582
		10 <sup>6</sup>	86	2495			10 <sup>6</sup>	86	2495
		10 <sup>7</sup>	82	2379			10 <sup>7</sup>	82	2379
		10 <sup>8</sup>	79	2292			10 <sup>8</sup>	79	2292
		10 <sup>9</sup>	76	2205			10 <sup>9</sup>	76	2205
		10 <sup>10</sup>	73	2118			10 <sup>10</sup>	73	2118
		10 <sup>11</sup>	70	2031			10 <sup>11</sup>	70	2031
		10 <sup>12</sup>	67	1944			10 <sup>12</sup>	67	1944
$\pi/2$	$\sqrt{2}$	10 <sup>3</sup>	98	2843	$\sqrt{2}$	$\pi/2$	10 <sup>3</sup>	98	2843
		10 <sup>4</sup>	94	2727			10 <sup>4</sup>	94	2727
		10 <sup>5</sup>	91	2640			10 <sup>5</sup>	91	2640
		10 <sup>6</sup>	87	2524			10 <sup>6</sup>	88	2524
		10 <sup>7</sup>	84	2437			10 <sup>7</sup>	84	2437
		10 <sup>8</sup>	81	2350			10 <sup>8</sup>	81	2350
		10 <sup>9</sup>	77	2234			10 <sup>9</sup>	78	2234
		10 <sup>10</sup>	90	2611			10 <sup>10</sup>	90	2611
		10 <sup>11</sup>	72	2089			10 <sup>11</sup>	72	2089
		10 <sup>12</sup>	103	2988			10 <sup>12</sup>	102	2959

TABLE 4

The time taken to compute Gauss-Jacobi quadrature rules of various orders via the algorithm of this paper, and the accuracy of the resulting rules. All times are in seconds. A maximum of 28 simultaneous threads of executions were allowed during these calculations.

Order (n)	$\gamma = -0.3, \quad \zeta = 0.25$			$\gamma = \pi/2, \quad \zeta = \sqrt{2}$		
	Phase function time	Quadrature time	Maximum relative error in weights	Phase function time	Quadrature time	Maximum relative error in weights
$10^3$	$5.14 \times 10^{-02}$	$1.02 \times 10^{-02}$	$8.49 \times 10^{-14}$	$4.98 \times 10^{-02}$	$3.55 \times 10^{-02}$	$3.59 \times 10^{-14}$
$10^4$	$4.75 \times 10^{-02}$	$3.31 \times 10^{-02}$	$8.19 \times 10^{-14}$	$6.59 \times 10^{-02}$	$5.07 \times 10^{-02}$	$4.01 \times 10^{-14}$
$10^5$	$4.62 \times 10^{-02}$	$3.85 \times 10^{-02}$	$2.07 \times 10^{-14}$	$4.70 \times 10^{-02}$	$2.51 \times 10^{-02}$	$1.43 \times 10^{-14}$
$10^6$	$4.41 \times 10^{-02}$	$3.92 \times 10^{-02}$	$3.64 \times 10^{-14}$	$4.37 \times 10^{-02}$	$3.91 \times 10^{-02}$	$2.24 \times 10^{-14}$
$10^7$	$4.13 \times 10^{-02}$	$2.17 \times 10^{-01}$	$5.21 \times 10^{-14}$	$4.10 \times 10^{-02}$	$2.59 \times 10^{-01}$	$3.68 \times 10^{-14}$
$10^8$	$4.22 \times 10^{-02}$	$2.07 \times 10^{+00}$	$5.87 \times 10^{-15}$	$4.29 \times 10^{-02}$	$2.01 \times 10^{+00}$	$1.76 \times 10^{-14}$
$10^9$	$3.95 \times 10^{-02}$	$1.82 \times 10^{+01}$	$3.99 \times 10^{-15}$	$3.95 \times 10^{-02}$	$1.99 \times 10^{+01}$	$3.52 \times 10^{-14}$
$10^{10}$	$4.24 \times 10^{-02}$	$1.85 \times 10^{+02}$	$4.28 \times 10^{-15}$	$5.07 \times 10^{-02}$	$1.85 \times 10^{+02}$	$1.10 \times 10^{-15}$
$10^{11}$	$3.77 \times 10^{-02}$	$1.76 \times 10^{+03}$	$6.57 \times 10^{-15}$	$3.81 \times 10^{-02}$	$1.84 \times 10^{+03}$	$1.29 \times 10^{-14}$
$10^{12}$	$3.65 \times 10^{-02}$	$1.78 \times 10^{+04}$	$4.54 \times 10^{-15}$	$6.39 \times 10^{-02}$	$1.87 \times 10^{+04}$	$9.99 \times 10^{-15}$

$(0, \pi/2]$  and those of  $z_n^{(\zeta, \gamma)}$  in the interval  $(0, \pi/2)$ . More specifically, if we denote by

$$\theta_1 < \theta_2 < \dots < \theta_{\lceil n/2 \rceil} \quad (99)$$

the roots of the function  $z_n^{(\zeta, \gamma)}$  in the interval  $(0, \pi/2]$  and by

$$\theta_{\lceil n/2 \rceil + 1} < \theta_{\lceil n/2 \rceil + 2} < \dots < \theta_n \quad (100)$$

the roots of  $z_n^{(\gamma, \zeta)}$  in the interval  $(0, \pi/2)$ , then the nodes of the  $n$ -point Gauss-Jacobi quadrature rule are given by the formula

$$t_j = \begin{cases} -\cos(\theta_j) & \text{if } 1 \leq j \leq \lceil \frac{n}{2} \rceil \\ \cos(\theta_{n-j+1}) & \text{if } \lceil \frac{n}{2} \rceil < j \leq n. \end{cases} \quad (101)$$

As in the case of Gauss-Legendre quadrature rules, the weights of Gauss-Jacobi quadrature rules can be expressed in terms of the derivatives of the phase functions which represent the functions  $z_n^{(\gamma, \zeta)}$  and  $z_n^{(\zeta, \gamma)}$ ; more specifically, we combine (21), (92) and (101) to obtain

$$w_j = \begin{cases} \frac{\Gamma(n + \gamma + 1)\Gamma(n + \zeta + 1)}{\Gamma(n + 1)\Gamma(n + \gamma + \zeta + 1)} \frac{(r^{(\zeta, \gamma)}(\theta_j))^2}{(d_1^{(\zeta, \gamma)})^2 \alpha^{(\zeta, \gamma)'(\theta_j)}} & \text{if } 1 \leq j \leq \lceil \frac{n}{2} \rceil \\ \frac{\Gamma(n + \gamma + 1)\Gamma(n + \zeta + 1)}{\Gamma(n + 1)\Gamma(n + \gamma + \zeta + 1)} \frac{(r^{(\gamma, \zeta)}(\theta_{n-j+1}))^2}{(d_1^{(\gamma, \zeta)})^2 \alpha^{(\gamma, \zeta)'(\theta_{n-j+1})}} & \text{if } \lceil \frac{n}{2} \rceil < j \leq n. \end{cases} \quad (102)$$

We follow [20] in using the asymptotic formula

$$\frac{\Gamma(\gamma + n)\Gamma(\zeta + n)}{\Gamma(\chi + n)\Gamma(\gamma + \zeta - \chi + n)} \approx 1 + \sum_{m=1}^M \frac{(-\gamma)_m(-\zeta)_m}{\Gamma(m+1)(-\gamma - \zeta - n)_m}, \quad (103)$$

which is a special case of (3.1) in [8], in order to evaluate the ratio of gamma functions appearing in (102). The symbol  $(x)_m$  appearing in (103) is the Pochhammer symbol, which is defined via

$$(x)_m = x(x+1)\dots(x+m). \quad (104)$$

We used the algorithm of Section 4 to construct Gauss-Jacobi rules of various orders  $n$  and for various values of  $\gamma$  and  $\zeta$ . We tested the accuracy of these rules by comparing the first  $\min\{10^7, n\}$  weights to those

generated by running the Glaser-Liu-Rokhlin [14] algorithm using IEEE quadruple precision arithmetic. Table 4 reports the results. For each combination of  $\gamma$ ,  $\zeta$  and  $n$  considered, it lists the time taken to compute the nonoscillatory phase functions representing  $z_n^{(\gamma, \zeta)}$  and  $z_n^{(\gamma, \zeta)}$  and their inverses, the total time required to calculate the nodes and weights of the corresponding Gauss-Jacobi quadrature rule, and the maximum relative error in the weights of that Gauss-Jacobi rule. A maximum of 28 simultaneous threads of execution were allowed during these calculations.

In Table 5, we compare the time required to compute Gauss-Jacobi quadratures rules of various orders using the algorithm of this paper with the time required to do so using the algorithm of [20]. The parameters were taken to be  $\gamma = 0.2$  and  $\zeta = 0.5$ . We used the adaptive version of our algorithm with  $k = 30$  and the Julia implementation [19] provided by the authors of [20]. These calculations were performed using a single processor core.

TABLE 5

*A comparison of the time taken to construct Gauss-Jacobi quadrature rules of various orders using the approach of this paper and the specialized approach of [20]. Here, the parameters were taken to be  $\gamma = 0.2$  and  $\zeta = 0.5$ . These computations were performed using a single processor core and all times are in seconds. Entries marked with a “—” indicate experiments which were prohibitively expensive to perform.*

Order	Algorithm of this paper	Algorithm of [20]
$10^3$	$5.58 \times 10^{-02}$	$3.22 \times 10^{-02}$
$10^4$	$5.50 \times 10^{-02}$	$1.65 \times 10^{-01}$
$10^5$	$8.63 \times 10^{-02}$	$1.29 \times 10^{+00}$
$10^6$	$4.72 \times 10^{-01}$	$1.14 \times 10^{+01}$
$10^7$	$3.13 \times 10^{+00}$	$2.03 \times 10^{+02}$
$10^8$	$2.92 \times 10^{+01}$	$2.03 \times 10^{+03}$
$10^9$	$2.89 \times 10^{+02}$	—
$10^{10}$	$2.82 \times 10^{+03}$	—

**5.4. Gauss-Laguerre quadrature formulas.** The Laguerre polynomial  $L_n^{(\gamma)}$  is a solution of the ordinary differential equation

$$t\psi''(t) + (1 + \gamma - t)\psi'(t) + n\psi(t) = 0 \text{ for all } 0 \leq t < \infty. \quad (105)$$

Its zeros  $t_1 < t_2 < \dots < t_n$  are the nodes of the Gauss-Laguerre quadrature rule

$$\int_0^\infty t^\gamma \exp(-t)f(t) dt \approx \sum_{k=1}^n f(t_k)w_k, \quad (106)$$

and the weights  $w_1, \dots, w_n$  are given by the formula

$$w_j = \frac{\Gamma(n + \gamma + 1)}{\Gamma(n + 1)} \frac{1}{t_j \left( L_n^{(\gamma)'}(t_j) \right)^2}. \quad (107)$$

Formula (107) can be found in many sources; it appears as (15.3.5) in [33], for instance. The function  $z_n$  defined via

$$z_n(u) = L_n(\exp(u)) \exp\left(-\frac{\exp(u)}{2} + \frac{\gamma u}{2}\right) \quad (108)$$

satisfies the second order differential equation

$$z''(u) + \left(\frac{\exp(u)}{2} - \frac{1}{4}(\gamma - \exp(u))^2 + \exp(u)n\right) z(u) = 0 \quad (109)$$

on the interval  $(-\infty, \infty)$  and the function

$$y_n(v) = L_n(v^2) \exp(-v^2/2) v^{1/2+\gamma} \quad (110)$$

is a solution of

$$y''(v) + \left(2 + 2\gamma + 4n + \frac{1 - 4\gamma^2}{4v^2} - v^2\right) y(v) = 0 \quad (111)$$

on the interval  $(0, \infty)$ .

For each of several values of  $n$  and  $\gamma$ , we used the algorithm of this paper to construct two nonoscillatory phase functions,  $\alpha_1$  and  $\alpha_2$ . The function  $\alpha_1$  represented solutions of (109) on the interval

$$(-30, 0.0), \quad (112)$$

and  $\alpha_2$  represented solutions of (111) on the interval

$$\left(\gamma, \sqrt{2n + \gamma - 2 + \sqrt{1 + 4(n-1)(n + \gamma - 1)}}\right), \quad (113)$$

where  $\zeta$  is the largest root of the Laguerre polynomial  $L_n^{(\gamma)}$  in  $(0, 1)$ . The interval (113) was chosen in light of the bound

$$t_n < 2n + \gamma - 2 + \sqrt{1 + 4(n-1)(n + \gamma - 1)}, \quad (114)$$

which can be found in [24]. The phase function  $\alpha_1$  representing solutions of (109) was constructed first; the values of  $z_n$  and its derivative at the point  $-30$ , which were used in order to obtain  $c_1$  and  $c_2$  such that

$$z_n(u) = c_1 \frac{\sin(\alpha_1(u) + c_2)}{\sqrt{\alpha_1'(u)}}, \quad (115)$$

were calculated using a 7-term Taylor expansion for the function

$$L_n(t) \exp\left(-\frac{t}{2}\right) t^{\gamma/2}. \quad (116)$$

The left endpoint of the interval (112) was chosen in lieu of a bound for the smallest root of  $L_n$  (of the sort appearing in [24]) in order to ensure the accuracy of these approximations. Once the coefficients  $c_1$  and  $c_2$  were obtained, we calculated the location of the largest root  $\zeta$  of  $z_n$  on the interval  $(0, 1)$  as well as the value of  $z'_n(\zeta)$ . These values were used to construct the coefficients  $d_1$  and  $d_2$  in the representation

$$y_n(v) = d_1 \frac{\sin(\alpha_2(v) + d_2)}{\sqrt{\alpha_2'(v)}} \quad (117)$$

of  $y_n$  in terms of the phase function  $\alpha_2$  for equation (111) on the interval (113). Note that, as discussed in Section 1, there is no need to evaluate trigonometric functions of large arguments in order to obtain the value of  $z'_n$  at  $\zeta$  (and hence none of the attendant loss of precision). We used two phase functions to represent  $L_n$  because some precision was lost when we represented  $L_n$  on an interval containing all of its zeros using a single phase function. The adaptive version of the algorithm of Section 4 was used to construct both phase

TABLE 6

*The time (in seconds) taken to compute Gauss-Laguerre quadrature rules of various orders via the algorithm of this paper, and the size of the expansions of the phase functions used to represent the solution. These calculations were performed using a single processor core.*

Order (n)	$\gamma = -0.5$		$\gamma = 0$		$\gamma = 0.5$	
	Phase function expansion size	Total time	Phase function expansion size	Total time	Phase function expansion size	Total time
$10^3$	8764	$2.37 \times 10^{-01}$	8212	$2.16 \times 10^{-01}$	8787	$2.29 \times 10^{-01}$
$10^4$	11938	$3.09 \times 10^{-01}$	11869	$3.11 \times 10^{-01}$	11892	$3.13 \times 10^{-01}$
$10^5$	12168	$3.90 \times 10^{-01}$	12168	$3.91 \times 10^{-01}$	12099	$3.94 \times 10^{-01}$
$10^6$	8741	$5.28 \times 10^{-01}$	8695	$5.10 \times 10^{-01}$	8419	$5.02 \times 10^{-01}$
$10^7$	4831	$2.71 \times 10^{+00}$	4785	$2.71 \times 10^{+00}$	2025	$2.66 \times 10^{+00}$
$10^8$	14744	$2.43 \times 10^{+01}$	10765	$2.39 \times 10^{+01}$	19114	$2.45 \times 10^{+01}$
$10^9$	23275	$2.52 \times 10^{+02}$	9802	$3.01 \times 10^{+02}$	5743	$3.42 \times 10^{+02}$

functions and the parameter  $k$  was taken to be 30.

For each pair of chosen values of  $n$  and  $\gamma$ , we computed the zeros  $u_1 < u_2 < \dots < u_k$  of  $z_n$  on the interval (113) and then used the formulas

$$t_j = \exp(u_j) \quad (118)$$

and

$$w_j = \frac{\exp(-\exp(u_j)) \exp((1 + \gamma)u_j)}{c_1^2 \alpha_1'(u_j)} \quad (119)$$

in order to construct the nodes of (106) in the interval  $(0, 1)$  and the corresponding weights. The expression (119) is obtained by combining (21), (107) and (108). We next computed the zeros  $v_1 < v_2 < \dots < v_{n-k}$  of  $y_n$  in the interior of the interval (113). The nodes  $t_{k+1} < t_{k+2} < \dots < t_n$  of the rule (106) contained in the interval  $(1, \infty)$  are related to those of  $y_n$  via the formula  $t_{k+j} = v_j^2$ , and the corresponding weights are given by

$$w_{k+j} = \frac{4 \exp(-v_j^2) v_j^{1+2\gamma}}{d_1^2 \alpha'(v_j)}. \quad (120)$$

Formula (120) is obtained in the usual fashion — by combining (21), (107) and (110).

Table 6 reports the results of these experiments; for each chosen pair of  $n$  and  $\gamma$ , it lists the total time required to compute the quadrature rule (including the time required to compute the phase function and its inverse), and the sum of the sizes of the expansions used to represent the two nonoscillatory phase functions. These calculations were performed using a single processor core.

**5.5. Roots of Bessel functions.** For each positive real number  $\nu$ , we denote by  $J_\nu$  the solution of Bessel's equation

$$t^2 y''(t) + t y'(t) + (t^2 - \nu^2) y(t) = 0 \quad \text{for all } 0 \leq t < \infty \quad (121)$$

which is finite at the origin. The function  $J_\nu$  has an infinite number of roots in the interval  $(\nu, \infty)$  on which it oscillates. The equation (121) is brought into the form

$$z''(u) + (\exp(2u) - \nu^2) z(u) = 0 \quad \text{for all } -\infty < u < \infty \quad (122)$$

via the transformation

$$z(u) = y(\exp(u)). \quad (123)$$

For various values of  $\nu$ , we constructed a nonoscillatory phase function  $\alpha$  representing solutions of (122) in the interval

$$\left[ \log(\nu), \log \left( \left( 10^9 + \frac{\nu}{2} - \frac{1}{4} \right) \pi \right) \right]. \quad (124)$$

The right endpoint in (124) is an upper bound for the location of the one billionth root of the function  $J_n(\exp(u))$  (see, for instance, 10.21.19 in [28]). The Equation (122) has a turning point at  $u = \log(\nu)$ ; consequently, any phase function representing its solutions is singular there. We used the adaptive version of the algorithm of Section 4 in order to construct phase functions in these experiments. The parameter  $k$  was taken to be 30.

The coefficients  $d_1$  and  $d_2$  such that

$$J_\nu(\exp(t)) = d_1 \frac{\sin(\alpha(t) + d_2)}{\sqrt{\alpha'(t)}} \quad (125)$$

were calculated using the approximations of the values of  $J_\nu$  and its derivative at the point  $\nu$  obtained via the formulas

$$J_\nu(\nu) = \frac{1}{\pi} \int_0^\pi \exp(-\nu F(t)) dt \quad (126)$$

and

$$J'_\nu(\nu) = \frac{1}{\pi} \int_0^\pi \frac{t - \sin(t) \cos(t)}{\sqrt{t^2 - \sin(t)^2}} \exp(-\nu F(t)) dt, \quad (127)$$

TABLE 7

The time (in seconds) taken to compute the first one billion roots of Bessel functions of various orders, the accuracy of the obtained roots, and the size of the piecewise expansion used to represent the associated nonoscillatory phase functions. A maximum of 28 simultaneous threads of execution were allowed during these calculations.

$\nu$	Phase function expansion size	Phase function time	Root calculation time	Maximum relative error
$\sqrt{2} \cdot 10^3$	2205	$2.89 \times 10^{-02}$	$8.58 \times 10^{+00}$	$1.83 \times 10^{-15}$
$\pi \cdot 10^4$	2305	$3.48 \times 10^{-02}$	$8.58 \times 10^{+00}$	$1.81 \times 10^{-15}$
$\pi \cdot 10^5$	2466	$3.19 \times 10^{-02}$	$8.63 \times 10^{+00}$	$3.89 \times 10^{-14}$
$\sqrt{3} \cdot 10^6$	2066	$3.00 \times 10^{-02}$	$8.48 \times 10^{+00}$	$1.59 \times 10^{-15}$
$\pi \cdot 10^7$	1770	$2.50 \times 10^{-02}$	$8.78 \times 10^{+00}$	$1.72 \times 10^{-15}$
$\sqrt{2} \cdot 10^8$	2466	$3.22 \times 10^{-02}$	$8.53 \times 10^{+00}$	$1.67 \times 10^{-15}$
$\pi \cdot 10^9$	3858	$4.99 \times 10^{-02}$	$8.97 \times 10^{+00}$	$4.06 \times 10^{-15}$
$\sqrt{3} \cdot 10^{10}$	4148	$5.01 \times 10^{-02}$	$1.06 \times 10^{+01}$	$1.65 \times 10^{-15}$

where

$$F(t) = \log \left( \frac{t + \sqrt{t^2 - \sin(t)^2}}{\sin(t)} \right) - \cot(t) \sqrt{t^2 - \sin(t)^2}. \quad (128)$$

Formulas (126) and (127) appear in Section 8.53 of [36], among many other sources. Note that the integrands in (126) and (127) are nonoscillatory so that the order of the quadrature rule needed to calculate them does not depend on  $\nu$ .

For each chosen value of  $\nu$ , we used the nonoscillatory phase function to compute the first one billion roots of  $J_\nu$ . The obtained values were compared against those generated by running the Glaser-Liu-Rokhlin algorithm [14] using IEEE quadruple precision arithmetic. Table 7 shows the results; it reports the number of values used to represent each nonoscillatory phase function, the time taken to construct each phase function, the time required to calculate the roots, and the maximum relative error in the obtained roots.

**6. Conclusions.** We have described a fast and highly accurate algorithm for the computation of the roots of special functions satisfying second order ordinary differential equations. Despite its great generality, when it is used to construct classical Gaussian quadrature rules our algorithm is competitive with specialized, state-of-the-art methods. It is based on two observations: (1) the solutions of second order linear ordinary differential equations of the form

$$y''(t) + q(t)y(t) = 0, \quad (129)$$

where  $q$  is smooth and positive, can be represented as

$$y(t) = \frac{d_1 \sin(d_2 + \alpha(t))}{\sqrt{\alpha'(t)}} \quad (130)$$

with  $\alpha$  a nonoscillatory function even when the magnitude of  $q$  is large, and (2) the roots of a function  $y$  represented in the form (130) and the values of its derivative  $y'$  at those roots can be calculated without evaluating trigonometric functions of large orders and the concomitant loss of precision.

Our algorithm was designed for reliability and accuracy at the expense of speed. It can be significantly accelerated, particularly in the case of moderate values of the parameter  $\lambda$ , and improvements in it will be reported by the author at a later date. As will algorithms for the fast evaluation of certain special functions and the fast application of the associated transforms which take advantage of the fact that explicit formulas for nonoscillatory phase functions are available in some cases.

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