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Modelling, Analysis and Simulation

Modelling, Analysis and Simulation

Algorithm 850: Real parabolic cylinder functions *U(a,x)*, *V(a,x)*

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ABSTRACT

Fortran 90 programs for the computation of real parabolic cylinder functions are presented. The code computes the functions $U(a, x)$, $V(a, x)$ and their derivatives for real a and x ($x \geq 0$). The code also computes scaled functions. The range of computation for scaled PCFs is practically unrestricted. The aimed relative accuracy for scaled functions is better than $5\,10^{-14}$. Exceptions to this accuracy are the evaluation of the functions near their zeros and the error caused by the evaluation of trigonometric functions of large arguments when $|a| >> x$. The routines always give values for which the Wronskian relation for scaled functions is verified with a relative accuracy better than $5\,10^{-14}$. The accuracy of the unscaled functions is also better than $5\,10^{-14}$ for moderate values of x and a (except close to the zeros), while for large x and a the error is dominated by exponential and trigonometric function evaluations. For IEEE standard double precision arithmetic, the accuracy is better than $5\,10^{-13}$ in the computable range of unscaled PCFs (except close to the zeros).

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Algorithm 850: Real Parabolic Cylinder Functions $U(a,x)$, $V(a,x)$

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Categories and Subject Descriptors: G.4 [**Mathematics of Computing**]: Mathematical software

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1. INTRODUCTION

The algorithm computes both functions $U(a,x)$ and $V(a,x)$, which constitute a satisfactory pair of independent solutions [2] of the differential equation

$$w'' - \left(\frac{x^2}{4} + a\right) w = 0, \tag{1}$$

and their derivatives. Also scaled functions can be computed which can be used for unrestricted values of a and x.

We refer to [2] for properties of $U(a,x)$ and $V(a,x)$ and for further details of the analytical and numerical aspects.

The algorithm combines different methods of evaluation in different regions.

Some of these methods share regions of validity. Comparison between the different methods, together with the use of the Wronskian relation and the recurrence relations, has been used to determine the accuracy of the algorithm (see Section 2). The relative accuracy for scaled functions is better than $5\,10^{-14}$ except, unavoidably, in the vicinity of the zeros of the functions, which take place in the oscillatory region $x^2/4 + a < 0$. Also in the vicinity of the (x, a)-points $(0, 2k - 1/2)$, $(0, 2k - 3/2)$, $k \in \mathbb{N}$, loss of relative precision is unavoidable for $V(a, x)$ and $V'(a, x)$ respectively because $V(2k - 1/2, 0) = 0$, $V'(2k - 3/2, 0) = 0$.

For scaled functions the Wronskian relation is verified with a relative accuracy better than $5\,10^{-14}$. The accuracy of the unscaled functions is also better than $5\,10^{-14}$ for moderate values of x and a (except close to the zeros), but for larger x and a the accuracy decreases mildly and it is dominated by exponential and trigonometric function evaluations. For IEEE standard double precision arithmetic, we have verified that the accuracy is better than $5\,10^{-13}$ in the computable range of unscaled PCFs (except close to the zeros)

2. REGIONS OF APPLICATION OF THE METHODS AND ACCURACY.

In order to determine the region of applicability of the each methods of computation described in [2], we have compared power series, asymptotic expansions (Poincaré-type, Airy-type and expansions in terms of elementary functions) and recurrence relations with the non-oscillating integral representations [1; 2]. These integrals are a valid method of computation for most of the (a, x)-plane (except for small a and for small x and positive a) and therefore they are an important tool in order to determine the regions of validity for the rest of the methods for a given accuracy. The selection of one method or another, when alternatives are available, will depend on the efficiency of each of these methods (see Section 5).

We provide the curves f_i, $i = 1, ..., 12$ appearing in Figure 1 together with the equations of two additional curves (f_{13} and f_{14}) which are outside of the represented domain. We use the notation $x_{i,j}$ to denote the x value for the intersection vertices of the curves f_i and f_j which appear in the figure.

$$
\begin{array}{ll}
f_1 : a = -0.23x^2 + 1.2x + 18.72, & 0 \le x \le x_{1,9} = 30 \\
f_2 : a = \frac{3.75}{x} - 1.25, & x_{1,2} \le x \le x_{2,3} = 3 \\
f_3 : a = -30/(x - 0.3) + 100/9, & x_{3,4} \le x \le x_{2,3} = 3 \\
f_4 : a = -0.21x^2 - 4.5x - 40, & 0 \le x \le x_{4,10} = 30 \\
f_5 : a = x - 14, & x_{5,12} = 4 \le x \le x_{5,6} \\
f_6 : a = -7 - 0.14(x - 4.8)^2, & x_{5,6} \le x \le x_{1,6} \\
f_7 : a = 2.5x - 30, & x_{1,7} = 12 \le x \le x_{7,13} = 72 \\
f_8 : a = -2.5x + 30, & x_{1,8} = 12 \le x \le x_{8,14} = 72 \\
f_9 : a = -0.1692x^2, & x > x_{1,9} = 30 \\
f_{10} : a = -0.295x^2 + 0.3x - 107.5, & x > x_{4,10} = 30 \\
f_{11} : a = 0, & x_{2,3} = 3 \le x \le x_{1,7} = x_{1,8} = 12 \\
f_{12} : x = 4, & x_{4,12} = -61.26 \le a \le -10 = x_{5,12} \\
f_{13} : a = 150 & x > x_{7,13} = 72 \\
f_{14} : a = -150 & x > x_{8,14} = 72
\end{array}
$$

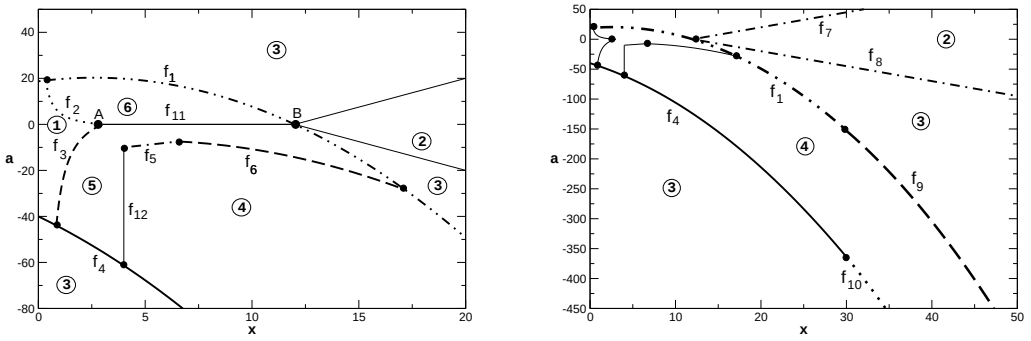

Figure 1. Regions in the (a, x)-plane where different methods of computation are considered. The curves f_i are plotted together with the intersection vertices between curves (black circles). The regions referred in the text are marked with numbered circles.

The values of $x_{1,2}$, $x_{3,4}$, $x_{5,6}$ and $x_{1,6}$ are (in double precision)

$$x_{1,2} = 0.1857815261497950$$

$$x_{3,4} = 0.8448329848762435$$

$$x_{5,6} = 6.5642426848523139$$

$$x_{1,6} = 17.151539704932772$$

With three exceptions, the curves shown in Figure 1 are all the curves separating the regions where different methods are applied. The first exception is related to the validity of Poincaré asymptotic expansions, which is not used for $|a| > 150$ (curves f_{13} and f_{14} which are outside the region depicted in Figure 1). The second exception is the rectangular region $|a| < 0.7$ and $x \in [2.5, 12.5]$, which includes the vertices A and B of Figure 1 (left); we will discuss later this particular case. The third exception is for positive a and small x (close to zeros of the V functions for positive a) where, as we describe later, uniform asymptotic expansions will be replaced by Maclaurin series for the V-functions.

Let us identify which are the methods used in each of the 8 regions in which the (a, x)-plane is divided by the 14 curves f_i. If not stated otherwise, the same method is applied for both $U(a, x)$ and $V(a, x)$ and their derivatives. Notice that the numbering of the methods in the following list corresponds to the labelling of the regions in Figure 1.

(1) Maclaurin series:
   (a) Bounded region delimited by the curves f_1, f_2, f_3 and f_4. Eqs. (14)-(16) and (17)-(19) of [2] are considered.

(2) Asymptotic expansions for large x (Poincaré type):
   (a) Unbounded region between $f_7 \cup f_{13}$ and $f_8 \cup f_{14}$ ($x > x_{7,8} = 12$). We apply Eqs. (23) and (26) of [2].

(3) Uniform asymptotic expansions in terms of elementary functions:
   (a) Unbounded region for positive a above the curves f_1, f_7 and f_{13} (f_{13} is not shown in Fig. 1). Eqs. (28) and (34) of [2] are applied.
   (b) Unbounded region for negative a between $f_8 \cup f_{14}$ and $f_1 \cup f_9$. Eqs. (28) and (39) of [2] are used.
   (c) Unbounded region for negative values of a below $f_4 \cup f_{10}$. Eqs. (40) and (43) of [2] are used.

(4) Uniform Airy-type asymptotic expansion:
   (a) Unbounded region for negative a delimited by the curves f_5, f_6, f_1 ($x \geq x_{1,6}$), f_9, f_{12}, f_4 ($x \geq x_{4,12}$) and f_{10}. Eqs. (56)-(59) of [2] are applied.

(5) Integral representations:
   (a) Bounded region for negative a encircled by the curves f_{11}, f_3, f_4 ($x_{3,4} \leq x \leq x_{4,12}$), f_{12}, f_5, f_6 and f_1 ($12 \leq x \leq x_{1,6}$). Eqs. (130)-(133) of [2] are used when $x^2/4 + a < 0$ with the modifications of Section 9.2.2 near $x^2/4 + a = 0$ and Eqs. (158)-(161) are considered when $x^2/4 + a > 0$).

(6) Series for V and recurrences for U
   (a) Bounded region for positive values of a encircled by the curves f_1, f_2 and f_{11}. Maclaurin series are used for V (Eq. (16) of [2]) and recurrence relations for U (Eqs. (68) and (70) of [2]) with starting values $a \in [21, 23)$ (computed with the uniform asymptotic expansions corresponding to the region 3).

Exceptions near $a = 0$: The above mentioned scheme is modified in the strip $|a| < 0.7$ and $x \in [2.5, 12.5]$ in order to avoid loss of accuracy of the integral representations when $|a|$ is small. For this purpose we apply recurrence relations for U in the strip. For the V function, Maclaurin series are considered in the strip when $2.5 \leq x \leq 10.5$, while recurrences are applied when $10.5 < x < 12.5$. Of course, the recurrence relation for the U and V functions are applied in the corresponding stable directions: backward for U and forward for V. The starting values for the recurrences are $a \in [21, 23)$ for U and $a \in (-22, -20]$ for V. These starting values are in the monotonic region $x^2/4 + a > 0$, where no zeros appear, and the starting values of $|a|$ are moderate, preventing overflow/underflow and bad conditioning.

Notice that this strip contains the (x, a)-points $\mathbf{A}(3,0)$ and $\mathbf{B}(12,0)$ in Figure 1. In this way we avoid the use of the asymptotic expansions in terms of elementary functions for too small a close to $\mathbf{B}$. It is worth noticing that the uniform asymptotic expansions in terms of elementary functions are valid even when a is small. This is not surprising given the double asymptotic property of the asymptotic expansions.

Exceptions near $x = 0$, $a > 0$: Because $V(2k - 1/2, 0) = V'(2k - 3/2, 0) = 0\,, k \in \mathbb{N}$, loss of accuracy is expected in the vicinity of the points $(x, a) = (0, k - 1/2)$. The loss of accuracy is better under control by considering Maclaurin series instead of asymptotic expansions for large a and small x. For this reason we consider series when $0 < a < 1/x^2$ and $0 \leq x < 0.005$.

As commented, the regions of application of each method have been selected by comparing each method with the integral representations, with the exceptions mentioned before. The next figures show these comparisons for a relative accuracy of $5\,10^{-14}$. For $a<0$ we test the modulus function

$$M(a,x)=\sqrt{\widetilde{U}(a,x)^2+2\pi\widetilde{V}(a,x)^2} \tag{2}$$

related to M_1 (see [2]), but with $\beta(|a|)$ substituted by 1. Also the analogous modulus function but with scaled derivatives can be considered:

$$N(a,x)=\sqrt{\widetilde{U'}(a,x)^2+2\pi\widetilde{V'}(a,x)^2}. \tag{3}$$

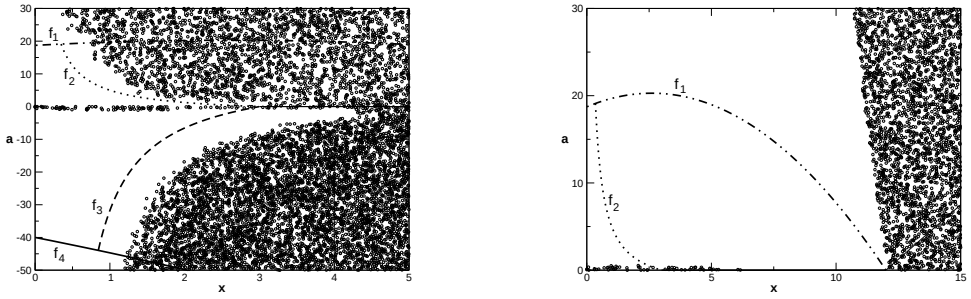

Figure 2. Comparison of McLaurin series against integral representations. The points where a $5\,10^{-14}$ relative accuracy is not reached are shown. In both cases, as explained in the text, integrals fail for small values of $|a|$. **Left**: the scaled U-function is tested for $a\geq 0$ and the modulus $M(x)$ for $a<0$. The region $[0,5]\times[-50,30]$ was sampled with 10^4 test points. **Right**: the V-function is tested. The region $[0,15]\times[0,30]$ was sampled with 10^4 test points.

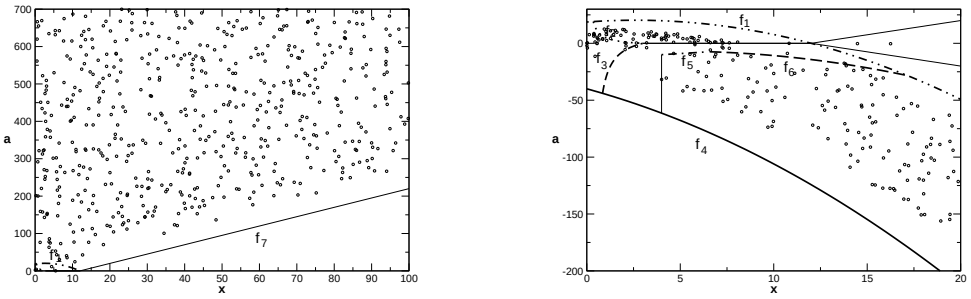

Figure 3. Comparison of two types of asymptotic expansions against integral representations. The points where a $5\,10^{-14}$ accuracy is not reached are shown. **Left**: Comparison of asymptotic expansions of Poincaré-type with integral representations for the scaled U- function. The region $[0,100]\times[0,1000]$ was sampled with 10^4 test points. Only part of the tested region is shown. **Right**: Comparison of asymptotic expansions in terms of elementary functions with integral representations. The region $[0,100]\times[-1000,30]$ was sampled with 10^4 test points. Only part of the tested region is shown.

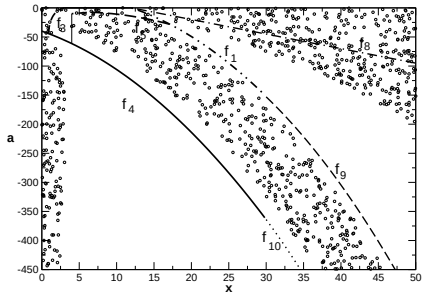

Figure 4. Asymptotic expansions in terms of Airy functions are tested against asymptotic expansions in terms of elementary functions. The modulus $M(a,x)$ is tested. The circles represent the points where a $5\,10^{-14}$ accuracy is not reached. Near the transition curve $x^2/4+a=0$, expansions in terms of elementary functions fail; away from the transition curve, the Airy-type expansions fail. The region $[0,100]\times[-1000,0]$ was sampled with 10^4 test points. Only part of the tested region is shown.

When the comparison with the integral representations was not possible, comparison with alternative software (Maple and the Fortran 77 code of ref. [2]) was considered. Also the Wronskian is used as a test. These combined numerical checks allow us to test the accuracy of the code in all regions of the (x,a)-plane. See Section 4 for further details.

3. OVERFLOW AND UNDERFLOW LIMITS

The scaled functions $\widetilde{U}$, $\widetilde{V}$, $\widetilde{U'}$, and $\widetilde{V'}$ do not have practical overflow/underflow limitations, because the dominant exponential factor $F(a,x)$ is scaled out. When computing plain (that is, unscaled) PCFs, the dominant exponential factor $F(a,x)$ is the source of overflows and underflows in the function values, the V-function and its derivative being proportional to $F(a,x)$ and U, and its derivative proportional to $F(a,x)^{-1}$.

In particular, we have $F(a,0)=|a|^{a/2}e^{-a/2}$ and then $F(a,0)\to+\infty$ as $a\to+\infty$ while $F(a,0)\to-\infty$ as $a\to-\infty$. In addition, $F(0,x)=e^{x^2/4}$ and $F(0,x)\to+\infty$ as $x\to+\infty$. This means that $V(a,x)$ will overflow for large positive $a>>x$ and for large $x>>a$ while it will underflow for negative a when $|a|>>x$ (the contrary happens for $U(a,x)$). Because $F(a,x)$ is a continuous function in the (a,x)-plane for $x\geq 0$, we expect that an infinite region should exist for $a<0$ where $V(a,x)$ does not overflow/underflow.

Figure 5 shows the curves for overflow/underflow limits taking $O=10^{300}$ as overflow number and $u=10^{-300}$ as underflow number. The curves follow from solving the equations $F(a,x)=O$ and $F(a,x)=u$.

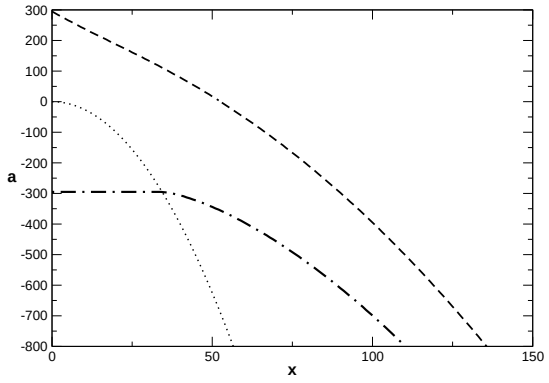

Figure 5. Overflow/underflow limits for an overflow number $O = 10^{300}$ and an underflow number $u = 10^{-300}$. Above the dashed line $F(a,x)$ overflows (and therefore V overflows while U underflows). Below the dashed-dotted line $F(a,x)$ underflows (and then V underflows while U overflows). The dotted line is the curve of turning points $a = -x^2/4$.

4. NUMERICAL TESTS

We have performed different types of numerical checks: we test Wronskian relations and recurrence relations and we compare quadrature against the full code and we also test recurrence relations. Comparison with other existing Fortran and Maple software has been also used.

4.1 Testing Wronskian relations

We test the Wronskian relation between $U(a,x)$ and $V(a,x)$:

$$\mathcal{W}[U(a,x),V(a,x)] = \sqrt{2/\pi}\,. \tag{4}$$

This is a numerically satisfactory test because, in any direction of the (a,x)-plane, when one of the functions is recessive the other one is dominant.

This expression also holds for the scaled functions $\widetilde{U}(a,x)$, $\widetilde{V}(a,x)$ if $x > 0$

We obtain the maximum relative errors for the Wronskian test using 10^8 random points in selected regions of the (x,a)-plane. For scaled functions we obtain:

(1) $[0,10]\times[-100,100]$: $3.3\,10^{-14}$,
(2) $[0,100]\times[-10000,10000]$: $2.9\,10^{-14}$,
(3) $[0,1000]\times[-100000,100000]$: $2.2\,10^{-14}$,

which is consistent with the $5\,10^{-14}$ accuracy claim. The fact that the errors obtained are smaller as larger regions are considered shows that the asymptotic expansions tend to be more accurate for large parameter values.

For unscaled functions, we repeat the analysis (but for narrower regions). For 10^8 random test points we obtain the following maximum relative errors:

(1) $[0,10]\times[-25,25]$: $3.7\,10^{-14}$,

(2) $[0,30]\times[-100,100]$: $7.4\,10^{-14}$,

(3) $[0,100]\times[-800,300]$: $2.5\,10^{-13}$,

which is consistent with the accuracy claim: $5\,10^{-13}$.

4.2 Testing quadrature against the full code

As described in [2] quadrature can be applied when $|a|$ is not very small. Also, when x is small, loss of accuracy is expected in the computation of V-values for semi-integer values of a. Apart from this, quadrature is a safe testing method for moderate values of the parameters. We compare the function values $\widetilde{U}(a,x)$, $\widetilde{U}'(a,x)$, $\widetilde{V}(a,x)$, and $\widetilde{V}'(a,x)$ in the monotonic region and for the oscillatory region we use the modulus functions $M(a,x)$ (Eq. (2)) and $N(a,x)$ (Eq. (3)).

We test the code against quadrature in the (x,a)region $[0,30]\times[-100,100]$ with 10^6 randomly generated points. The following results are obtained:

(1) When the values $|a|<1$ are excluded, the maximum relative error for the scaled U-functions in the monotonic region are $2.4\,10^{-14}$ for $\widetilde{U}$, $2.8\,10^{-14}$ for $\widetilde{U'}$. For the unscaled functions the maximum errors are $9.3\,10^{-14}$ for U and $9.3\,10^{-14}$ for U', consistently with the accuracy claims.

(2) When, apart from the values $|a|<1$, we also exclude $x<0.05$ when $a>0$, the maximum error for the V values in the monotonic region is: $2.7\,10^{-14}$ for $\widetilde{V}$, $2.2\,10^{-14}$ for $\widetilde{V'}$, $8.3\,10^{-14}$ for V and $8.3\,10^{-14}$ for V'.

(3) In the oscillatory region we test the moduli $M(a,x)$ and $N(a,x)$ when $a<-1.2$ (using the Wronskian relation we observe that the integrals lose some accuracy for $|a|<1.2$ in the oscillatory region). The maximum relative error obtained is $1.6\,10^{-14}$ for M and $1.1\,10^{-14}$ for N.

Naturally, the test gives no information on the accuracy in the regions where integrals are used in our code. Apart from this and the regions $|a|<1$, $-1.2<a<-1$ when $x<2$, and $x<0.05$ when $a>0$, integral representations give a direct check of function values from which the aimed accuracy can be verified.

In the last of these three regions, loss of accuracy is unavoidable for the V-functions near semi-integer values of a. However, because the U- functions are accurately computed and the Wronskian relations are verified, we can be confident on the accuracy of the code.

The remaining regions can be checked by testing the recurrence relations and by comparing with available software.

4.3 Testing recurrence relations against the full code

We compare the values of $V(a,x)$ computed directly from the code with the value obtained by applying the recurrence relation using the values of the contiguous functions $V(a-1,x)$ and $V(a-2,x)$. Also, we compute the $V'(a,x)$ from $V(a,x)$ and $V(a-1,x)$ and using Eq. (70) of [2]. We proceed similarly with the recurrence for U (but in the opposite direction) and with the relation of the derivatives with the contiguous functions. As before, in the oscillatory region we compute moduli functions (Eqs. (2) and (3)) for comparison. The recurrence test can only be applied for plain (unscaled) functions.

We compare the function values ($U(a,x)$, $U'(a,x)$, $V(a,x)$, $V'(a,x)$) in the monotonic region and the moduli functions $M(a,x)$, $N(a,x)$ in the oscillatory region. In the (x,a)-region $[0,30]\times[-100,100]$ and with 10^8 random test points we obtain the following results for the maximum relative error:

(1) In the monotonic region:
   (a) $1.9\,10^{-13}$ for $U(a,x)$,
   (b) $4.3\,10^{-13}$ for $U'(a,x)$,
   (c) $2.0\,10^{-13}$ for $V(a,x)$ when values $0<x<0.005$ are excluded for $a>0$,
   (d) $5.9\,10^{-13}$ for $V'(a,x)$ when values $0<x<0.005$ are excluded for $a>0$.

(2) In the oscillatory region:
   (a) $1.2\,10^{-13}$ for $M(a,x)$,
   (b) $2.5\,10^{-13}$ for $N(a,x)$.

We observe that the test for $V'(a,x)$ is slightly over the claimed accuracy. However, this is due to instabilities in the application of the relation for $V'(a,x)$ for large values of x close to the curve $a=-x^2/4$ in the monotonic region. It is observed that the two terms on the right of Eq. (70) of [2] tend to cancel. Let us recall that the Wronskian check is well below the limit of the accuracy claim.

4.4 Comparison with existing software

We compare the results from our code with the Maple functions CylinderU(a,x), CylinderV(a,x) and their corresponding derivatives in order to check the accuracy of our code in the parameter region $x\in[0,12]$, $a\in[-1,1]$, together with $-1.2<a<-1$ when $x<2$. For these parameter values, we do not compare our code against quadrature because they tend to fail for small values of $|a|$. We use 50 digits in the Maple computations.

The rectangle $x\in[2,12]$, $|a|<1$ is inside the monotonic region, where the direct comparison between functions is a valid test. With 10^4 tests in this region, the maximum errors found are: $2.0\,10^{-14}$ for $U(a,x)$; $2.0\,10^{-14}$ for $U'(a,x)$; $6.3\,10^{-16}$ for $V(a,x)$; $2.7\,10^{-14}$ for $V'(a,x)$.

We also test the moduli $M(a,x)$ and $N(a,x)$ in the (x,a)- region $[0,12]\times[-1.2,1.2]$ with 10^4 test points. Both functions agree with the results from Maple with a relative precision of $1.9\,10^{-14}$.

In addition, we compare our code against the codes DINPCF.F and DHAPCF.F of reference [3], which compute the functions $U(a,x)$, $V(a,x)$ for positive integer and half- integer values of a. The relative accuracy claim for these routines is better than 10^{-12}. We have compared the function values $U(a,x)$ and $V(a,x)$ using our code against DHAPCF.F (which computes $U(a,x)$ and $V(a,x)$ for positive half-integers values of a). For 10^6 random points and $x\in[0,30]$ (the range of a being the maximum available for DHAPCF.F), the maximum error found is $3.4\,10^{-13}$ for $U(a,x)$ and $1.4\,10^{-13}$ for $V(a,x)$. For integer values of a, comparison with DINPCF.F gives the following maximum relative errors: $3.5\,10^{-13}$ for $U(a,x)$ and $1.4\,10^{-13}$ for $V(a,x)$. These errors are consistent with the claim of accuracy for DHAPCF.F and DINPCF.F.

5. TIMING

In the following we show the CPU times (in seconds) spent by the code in representative regions where the different methods used for building the algorithm are applied. These CPU times refer to a PC with Pentium IV 2.8GHz processor and 1GB RAM running under Windows; the compiler used was the GNU Fortran compiler g95.

We provide the CPU-times spent for 10^6 evaluations in randomly chosen points of each of the selected regions. The results are:

(1) Series: $(x, a) \in [0, 1] \times [-20, 5]$, 6.99s.
(2) Uniform asymptotic expansions in terms of elementary functions for positive a: $(x, a) \in [10, 20] \times [30, 100]$, 5.78s.
(3) Series ($V(a, x)$) and recurrences ($U(a, x)$): $(x, a) \in [4, 8] \times [1, 12]$, 25.99s.
(4) Poincaré asymptotic expansion: $(x, a) \in [20, 60] \times [-10, 10]$, 3.05s.
(5) Integrals: $(x, a) \in [1.5, 3] \times [-40, -20]$, 320.54s.
(6) Uniform asymptotic expansions in terms of elementary functions for negative a and $x^2/4 + a > 0$: $(x, a) \in [40, 50] \times [-200, -150]$, 3.52s.
(7) Uniform Airy-type asymptotic expansions: $(x, a) \in [15, 25] \times [-150, -100]$, 33.63s.
(8) Uniform asymptotic expansions in terms of elementary functions for negative a and $x^2/4 + a < 0$: $(x, a) \in [0, 2.5] \times [-120, -60]$, 6.13s.

The following data correspond to CPU times (again for 10^6 points) spent by the full code:

(1) $(x, a) \in [0, 50] \times [-100, 100]$, 22.12s,
(2) $(x, a) \in [0, 1000] \times [-1000, 1000]$, 8.13s.

The algorithm has been tested in several computers and operating systems (Pentium IV PC under Windows XP and Red Hat Linux; Pentium IV laptop under Windows XP) and compilers (g95 for Linux and Windows, Digital Fortran for Windows).

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