Algorithm 914: Parabolic Cylinder Function $W(a, x)$ and its derivative

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A Fortran 90 program for the computation of the real parabolic cylinder functions $W(a, \pm x)$, $x \geq 0$ and their derivatives is presented. The code also computes scaled functions for $a > 50$. The functions $W(a, \pm x)$ are a numerically satisfactory pair of solutions of the parabolic cylinder equation $y'' + \left(x^2/4 - a\right) y = 0\,, \quad x \geq 0$. Using Wronskian tests, we claim a relative accuracy better than $5\,10^{-13}$ in the computable range of unscaled functions, while for scaled functions the aimed relative accuracy is better than $5\,10^{-14}$. This code, together with the algorithm and related software described in [5; 6], completes the set of software for parabolic cylinder functions (PCFs) for real arguments.

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

General Terms: Algorithms

Additional Key Words and Phrases: Parabolic cylinder functions, ODE integration, asymptotic expansions

1. INTRODUCTION

We present a Fortran 90 code for computing the Weber parabolic cylinder function $W(a, x)$ and its derivative. The parabolic cylinder function $W(a, x)$ [13, §12.14] is a solution of the differential equation

$$y'' + \left(\tfrac{1}{4}x^2 - a\right) y = 0\,, \quad x \geq 0. \tag{1}$$

which also has $W(a, -x)$ as a solution, the pair $\{W(a, x), W(a, -x)\}$ being a numerically satisfactory pair of solutions in the sense of Miller [9; 10].

The algorithm is based on the use, in different regions, of different methods of computation: Maclaurin series, local Taylor series, uniform asymptotic expansions in terms of elementary functions and Airy-type asymptotic expansions. All these methods are described in detail in [4].

The code gives as output the values of $W(a,x)$, $W(a,-x)$, $W'(a,x)$ and $W'(a,-x)$ for real a and $x \geq 0$. Notice that $W'(a,-x)$ is not exactly the derivative of $W(a,-x)$, but $W'(a-x) = -\frac{d}{dx}W(a,-x)$.

2. DEFINITION OF SCALED FUNCTIONS

For large (positive) values of the parameter a the functions $W(a,x)$, $W(a,-x)$ are very large or very small. To avoid overflow or underflow in numerical computations it is quite useful to define scaled values with the dominant exponential behavior factored out [7, sect. 12.1.3]. This scaling factor can be also factored out from the uniform asymptotic expansions.

We define the scaling factor as $e^{\chi(a,x)}$ where $\chi(a,x)$ is given by

$$\chi(a,x) = \begin{cases} a\left(\arcsin t + t\sqrt{1-t^2}\right), \text{ if } t \leq 1 \text{ (Monotonic Region)} \\ a\pi/2, \text{ if } t > 1 \text{ (Oscillating Region)} \end{cases} \tag{2}$$

with $t = x/(2\sqrt{a}) > 0$. For $a < 0$ scaling is not needed. We consider only positive values of x, which is not a restriction because we compute the pair $\{W(a,x), W(a,-x)\}$ and its derivatives.

The scaled functions are defined as

$$\begin{aligned} \widetilde{W}(a,x) &= e^{\chi(a,x)}W(a,x)\,, \quad \widetilde{W'}(a,x) = e^{\chi(a,x)}W'(a,x)\,, \\ \widetilde{W}(a,-x) &= \frac{W(a,-x)}{e^{\chi(a,x)}}\,, \quad \widetilde{W'}(a,-x) = \frac{W'(a,-x)}{e^{\chi(a,x)}}\,. \end{aligned} \tag{3}$$

Scaling factors can be directly factored out from the expressions used for the asymptotic expansions but not from the differential equation (1), which is the starting point of the local Taylor series method; because of this and in order to avoid introducing numerical errors due to the exponential terms of the scaling, scaled functions are computed for $a > 50$.

In particular and in the case of the Airy-type asymptotic expansions in the monotonic region ($t \leq 1$), the scaled functions $\widetilde{W}(a,\pm x)$ can be written in terms of scaled Airy-functions:

$$\widetilde{W}(a,x) \sim \frac{\pi^{\frac{1}{2}}\mu^{\frac{1}{3}}\ell(\mu)\phi(\zeta)}{2^{\frac{1}{2}}}\left(\widehat{\mathrm{Bi}}(-z)A_\mu(\zeta) + \frac{\widehat{\mathrm{Bi}}'(-z)}{\mu^{\frac{8}{3}}}B_\mu(\zeta)\right), \tag{4}$$

$$\widetilde{W'}(a,x) \sim -\frac{\pi^{\frac{1}{2}}\mu^{\frac{2}{3}}\ell(\mu)}{2e^{\frac{1}{2}}\phi(\zeta)}\left(-\frac{\widehat{\mathrm{Bi}}(-z)}{\mu^{\frac{4}{3}}}C_\mu(\zeta) + \widehat{\mathrm{Bi}}'(-z)D_\mu(\zeta)\right), \tag{5}$$

$$\widetilde{W}(a,-x) \sim \frac{\pi^{\frac{1}{2}}\mu^{\frac{1}{3}}\ell(\mu)\phi(\zeta)}{2^{-\frac{1}{2}}}\left(\widehat{\mathrm{Ai}}(-z)A_\mu(\zeta) + \frac{\widehat{\mathrm{Ai}}'(-z)}{\mu^{\frac{8}{3}}}B_\mu(\zeta)\right), \tag{6}$$

$$\widetilde{W'}(a,-x) \sim \frac{\pi^{\frac{1}{2}}\mu^{\frac{2}{3}}\ell(\mu)}{\phi(\zeta)}\left(-\frac{\widehat{\mathrm{Ai}}(-z)}{\mu^{\frac{4}{3}}}C_\mu(\zeta) + \widehat{\mathrm{Ai}}'(-z)D_\mu(\zeta)\right), \tag{7}$$

where $a=\frac{1}{2}\mu^2$, $z=\mu^{\frac{4}{3}}\zeta$, and for ζ we have the relation

$$\begin{cases} \frac{2}{3}(-\zeta)^{\frac{3}{2}} = \frac{1}{2}\arccos t - \frac{1}{2}t\sqrt{1-t^2}, & -1<t\le 1, \quad \zeta\le 0, \\ \frac{2}{3}\zeta^{\frac{3}{2}} = \frac{1}{2}t\sqrt{t^2-1} - \frac{1}{2}\ln\left(t+\sqrt{t^2-1}\right), & 1\le t, \quad \zeta\ge 0. \end{cases} \tag{8}$$

The function $\phi(\zeta)$ is given by $\phi(\zeta)=\left(\frac{\zeta}{t^2-1}\right)^{\frac{1}{4}}$ and $\ell(\mu)$ is computed by means of the asymptotic expansion

$$\ell(\mu)\sim \frac{2^{\frac{1}{4}}}{\mu^{\frac{1}{2}}}\sum_{s=0}^{\infty}\frac{\ell_s}{\mu^{4s}}, \tag{9}$$

where the first few coefficients are $\ell_0=1$, $\ell_1=-\frac{1}{1152}$, $\ell_2=-\frac{16123}{398\,13120}$, $\ell_3=-\frac{26954\,47331}{481\,57949\,95200}$, $\ell_4=-\frac{3759\,87489\,96091}{221\,91183\,33788}$.

Also, the computation of the functions $A_\mu(\zeta)$, $B_\mu(\zeta)$, $C_\mu(\zeta)$, and $D_\mu(\zeta)$ appearing in equations (4), (5), (6) and (7) is performed by using asymptotic expansions of the form

$$\begin{aligned} A_\mu(\zeta)&\sim\sum_{s=0}^{\infty}(-1)^s\frac{a_s(\zeta)}{\mu^{4s}}, \quad B_\mu(\zeta)\sim\sum_{s=0}^{\infty}(-1)^s\frac{b_s(\zeta)}{\mu^{4s}}, \\ C_\mu(\zeta)&\sim\sum_{s=0}^{\infty}(-1)^s\frac{c_s(\zeta)}{\mu^{4s}}, \quad D_\mu(\zeta)\sim\sum_{s=0}^{\infty}(-1)^s\frac{d_s(\zeta)}{\mu^{4s}}. \end{aligned} \tag{10}$$

Details on the coefficients a_s, b_s, c_s and d_s can be found in [12, §3.1].

Scaled Airy functions [8] are defined for $x>0$ as

$$\begin{aligned} \widehat{\mathrm{Ai}}(x)&=e^{\frac{2}{3}x^{3/2}}\mathrm{Ai}(x)\,, \quad \widehat{\mathrm{Ai}'}(x)=e^{\frac{2}{3}x^{3/2}}\mathrm{Ai}'(x)\,, \\ \widehat{\mathrm{Bi}}(x)&=e^{-\frac{2}{3}x^{3/2}}\mathrm{Bi}(x)\,, \quad \widehat{\mathrm{Bi}'}(x)=e^{-\frac{2}{3}x^{3/2}}\mathrm{Bi}'(x)\,, \end{aligned} \tag{11}$$

while $\widehat{\mathrm{Ai}}(x)=\mathrm{Ai}(x)$ when $x<0$ and the same applies for the derivative and for $\mathrm{Bi}(x)$ and its derivative.

The module for the computation of Airy functions uses a Fortran 90 version of the code by Fullerton [3] (the Fortran 77 code is available at Netlib).

3. REGIONS OF APPLICABILITY OF THE METHODS AND TESTING.

The curves f_i, $i=1,...,6$ appearing in Figures 1 and 2 correspond to the fitting curves separating regions of applicability of the methods. Explicit expressions for these curves are given by:

$$\begin{aligned} &f_1: \ a=7(x-2)^2+2.5 \text{ if } x<2; x=2 \text{ and } 0\le a\le 2.5 \\ &f_2: \ a=1.1x^2+30.5, \\ &f_3: \ a=0.2(x-12)^2+33, \\ &f_4: \ a=0.22x^2-40, \\ &f_5: \ a=-2(x-4.6)^2-3 \text{ if } f_5>f_6 \text{ and } x<3.8; \\ &\qquad a=-4 \text{ and } 3.8\le x\le 4.5; x=4.5 \text{ and } -4<a\le 0 \\ &f_6: \ a=0.13x^2-25 \end{aligned}$$

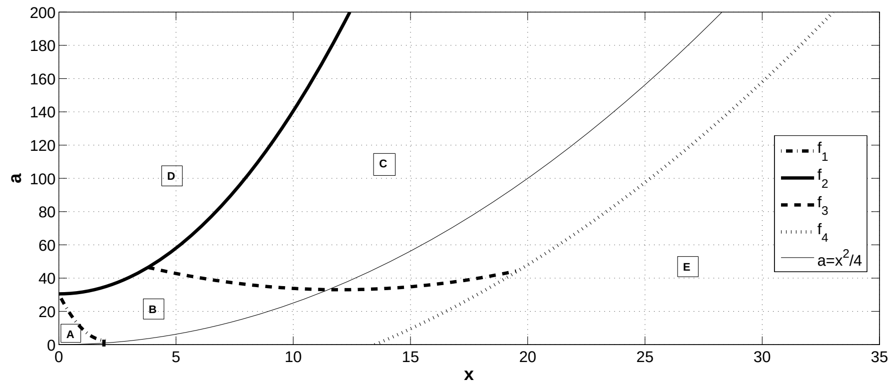

Figure 1. Regions in the (a,x)-plane $(a>0)$ where different methods of computation are considered. The curve $a=x^2/4$, frontier between the monotonic $(a>x^2/4)$ and the oscillatory $(a<x^2/4)$ behaviour of the functions, is also shown. The methods used are: **A)** Maclaurin series; **B)** Local Taylor series; **C)** Airy expansions; **D),E)** Expansions in terms of elementary functions.

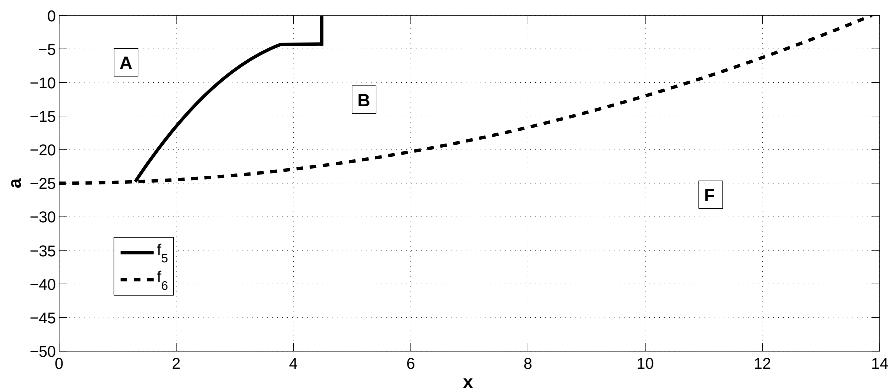

Figure 2. Regions in the (a,x)-plane $(a<0)$ where different methods of computation are considered. The methods used are: **A)** Maclaurin series; **B)** Local Taylor series; **F)** Asymptotic expansions for $a<0$.

3.1 Wronskian tests

We test the Wronskian relation between $W(a,x)$ and $W(a,-x)$, which is given by

$$\mathcal{W}[W(a,x),W(a,-x)]=1. \tag{12}$$

This relation means that

$$W(a,x)W'(a,-x)+W'(a,x)W(a,-x)=-1. \tag{13}$$

We compute the maximum relative errors for the Wronskian test using 10^7 random points in selected regions of the (x,a)-plane. For unscaled functions we obtain:

(1) $[0,100]\times[0,200]$: $1.5\,10^{-13}$,
(2) $[0,10000]\times[0,200]$: $1.22\,10^{-13}$,
(3) $[0,100]\times[-1000,0]$: $1.7\,10^{-13}$,
(4) $[0,1000]\times[-10000,0]$: $1.4\,10^{-13}$,
(5) $[0,10000]\times[-100000,0]$: $5.5\,10^{-14}$,

For scaled functions, the results for the Wronskian test are

(1) $[0,100]\times[50.01,1000]$: $1.1\,10^{-14}$,
(2) $[0,1000]\times[50.01,10000]$: $9\,10^{-15}$,

Based on these Wronskian tests, we claim an accuracy better than 5×10^{-13} in the computable range of unscaled functions and a relative accuracy better than 5×10^{-14} for scaled functions.

4. COMPARISON WITH EXISTING SOFTWARE

To our knowledge, no reliable (refereed) software is available for computing the functions $W(a,\pm x)$. A few algorithms have been described in [1; 11] with a claimed accuracy not better than eight digits. But according to the Digital Library of Mathematical Functions [2], the only existing routines are those included in the book [14]. However, these routines are built for a very limited range of validity (only $0<a<5$, $0<x<5$) Complex variable computations for the $W(a,\pm x)$ functions are available in Maple (or Mathematica) through complex confluent hypergeometric functions, but for large values of the parameters, and particularly for computing $W(a,x)$ for large $a>0$, these are very inefficient in comparison with the Fortran 90 calculations provided, because the representation of $W(a,x)$ in terms of confluent hypergeometric functions becomes unstable [4].

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