Fast Computation of the Complex Error Function

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1. Introduction

The complex error function $w(z) = \exp(-z^2)\left[1 + 2i/\sqrt{\pi}\int_0^z \exp(t^2)dt\right]$ of a complex variable $z = x + iy$ occurs in many branches of mathematics and physics. Rather abundant also are the methods for evaluating this function, from tables [1, 2] to modern software [3-5]. This function is particularly common in the plasma physics, since its computation is a necessary ground of the ion cyclotron resonance wave analysis in the laboratory fusion plasmas. Routinely, in applications this function is evaluated massively, therefore the efficiency of involved numerical algorithm is of primary importance.

At present time the algorithm 380 [3, 4] is the most successful, and most of the program libraries contain this algorithm. Jacobi's continued fraction

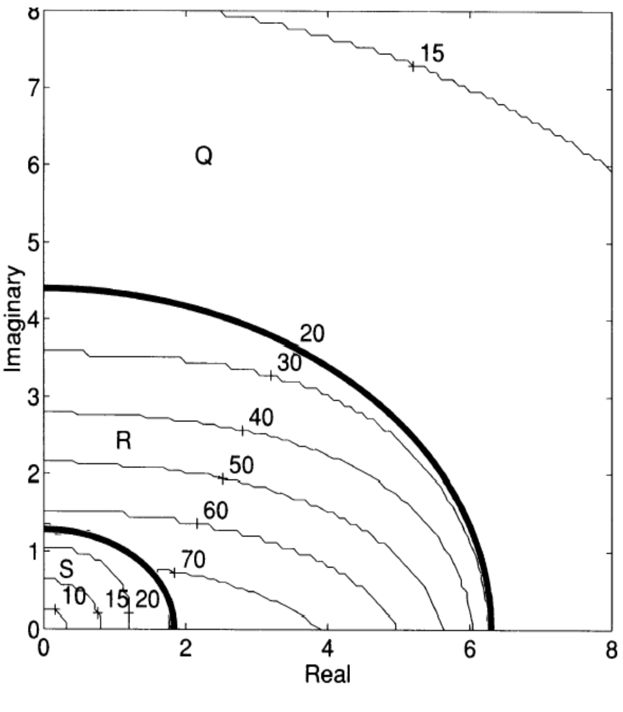
$$w(z) = \frac{1}{z-}\,\frac{1/2}{z-}\,\frac{1}{z-}\,\frac{3/2}{z-}\ldots$$

has been proved to provide the fast calculation of the complex error function by means of this method for large-$|z|$ values (Region Q, Fig.1). The same continued fraction with the Taylor expansion along the negative direction of the imaginary axis has been exploited for moderate-$|z|$ values (Region R, Fig.1). The Taylor expansion at the zero point

$$w(z) = \exp(-z^2)\left(1 + \frac{2i}{\sqrt{\pi}}\sum_{n=0}^{+\infty}\frac{z^{2n+1}}{(2n+1)\,n\,!}\right)$$

has been used for small-$|z|$ values (Region S, Fig.1). This method provides the accuracy up to 14 significant digits and the average computational time of the single function value approximately equals to 10 times for the single computation of the exponential function. From the standpoint of the computational time this method is most cheap (10-20 Arbitrary Units) in the

Fig.1.Efficiency of Gautschi's algoritm 680



regions S and Q and most expensive (30-70 Arbitrary Units) in the Region R. The main purpose of the present work is an attempt to clarify the issue of maximum possible efficiency to evaluate this function in the most problematic region R. Also, for calculations in this region we try to modify in order to accelerate the algorithm [3, 4] as far as possible.

2. **Computational procedure**

2.1 Algorithm 380

For evaluation of the complex error function $w(z)$ at the point z of the region R it was suggested to use a truncated Taylor expansion of this function at the point $z_0 = z + ih$ [3]

$$w(z) = \sum_{n=0}^{N} \frac{w^{(n)}(z+ih)}{n!}(-ih)^n \quad , \tag{1}$$

where $h > 0$ is suitably chosen. The expression (1) can be written in the form:

$$w(z) = \sum_{n=0}^{N} (2h)^n \, w_n(z+ih). \tag{2}$$

A ratio of two successive functions $r_{n-1} = w_n(z+ih)/w_{n-1}(z+ih)$ can be then developed into the continued fraction

$$r_{n-1} = \frac{1/2}{h - iz + (n+1)r_n}. \qquad n = 0, 1, 2, \ldots , \tag{3}$$

The method [3] uses the fact that at the one end of this continued fraction these ratios rather quickly tend to zero, if point $z_0 = z + ih$ is not close to abscissa axis. For this reason, this continued fraction can be truncated for the some finite value of the index $n = \nu > N$, and the last ratio can be put to zero $(r_\nu = 0)$. It can be shown that the sum in (2) can be recursively ($n = N, N-1 \ldots, 0$) calculated through

$$s_{n-1} = r_{n-1}\left[(2h)^n + s_n\right], \tag{4}$$

where $s_N = 0$ and $w(z) = 2/\sqrt{\pi} \cdot s_{-1}$. The choice of h affects both the convergence of the fraction (3) so and the convergence of the expansion (2). In fact, large values of h give rise to fast convergence of fraction (3), but slow convergence in (2), while small values of h yield slow convergence of (3), but fast convergence in (2). A good choice of h is therefore one which strikes a balance between these two opposing effects. This compromise value, corresponding to accuracy up to 10 significant digits, is $h = 1.6$ (Gautschi) and for accuracy up to 14 significant digits is $h = 1.88$ (Poppe&Wijers). In this algorithm, such a compromise in the choice of h corresponds to the optimum efficiency of the function evaluation and, consequently, the issue of the further algorithm improvement seems totally exhausted.

2.2 One more algorithm

However, instead the expansion (1), which is performed strictly along the imaginary axis, one can also use a more general expansion

$$w(z) = \sum_{n=0}^{N} \frac{w^{(n)}(z_0)}{n!}(z - z_0)^n \ , \tag{5}$$

and, instead the Gautschi functions $w_n(z)$, introduce a set of the functions $\varphi_n(z)$, related to the derivatives $w^{(n)}(z)$ by means of relations

$$w^{(n)}(z) = (2e^{-\varphi})^n n!\varphi_n(z) \ , \qquad (n = 0, 1, 2, \dots). \tag{6}$$

Here φ is related to $z - z_0$ in (5) as $z - z_0 = a e^{i\varphi}$ ($a = \sqrt{(x - x_0)^2 + (y - y_0)^2}$). It is easy to see that for $\varphi = -\pi/2$ it is true $\varphi_n(z) = w_n(z)$. The expansion (5) has then the form

$$w(z) = \sum_{n=0}^{N} \varphi_n(z_0)(2a)^n . \tag{7}$$

These functions satisfy to the recursive relation of 2nd order

$$\varphi_{n+1}(z_0) + \frac{z_0 e^{i\varphi}}{n+1}\varphi_n(z_0) + \frac{e^{2i\varphi}}{2(n+1)}\varphi_{n-1}(z_0) = 0 \ , \qquad n = 0, 1, 2, \dots ,$$

where the relations $\varphi_0(z_0) = w(z_0)$ and $\varphi_{-1} = -i2e^{-i\varphi}/\sqrt{\pi}$ are true . A ratio of two those successive functions $r^{\varphi}_{n-1} = \varphi_n(z_0)/\varphi_{n-1}(z_0)$ can be developed into recursive relation of the type (3)

$$\cdots r^{\varphi}_n = -\frac{e^{i\varphi}}{n+1}\left[z_0 + \frac{1/2\, e^{i\varphi}}{r^{\varphi}_{n-1}} \right] \cdots \qquad n = 0, 1, 2, \dots , \tag{8}$$

If one assumes that the value of the function $\varphi_0(z_0) = w(z_0)$ is known, it will be also known the ratio $r^{\varphi}_{-1} = \varphi_0(z_0)/\varphi_{-1}$. On the base the recursive relation (8) can be evaluated r^{φ}_n with indexes $n = 0, 1, \dots , N-1,$ respectively.

This way has some advantages in comparison with the previous algorithm. In first, coefficients of the fraction (8) in this case are calculated exactly, or rather with an accuracy of the starting ratio r^{φ}_{-1} or the function $w(z_0)$. Hence the choice of a is not limited to compromise mentioned above, and can be entirely subordinated to more efficient computing, namely, reduction the number of terms of the series (2).

Secondly, the expansions (1, 2) can be performed not only strictly along the imaginary axis, but along the somewhat direction to this favorable axis as well. The test calculations have showed that the maximum deviation angle should not significantly differ from the angle $-\pi/2$. These features allow one to construct a strategy of computing that significantly reduces the number of terms in the sum (7).

The region R is covered by a grid with the variable step a. The step size is chosen inversely proportional to the cost of computing time for evaluation of the function $w(z)$, presented in Fig.1. For area of R below the line with the number 70 is a step is 20/70, where the number 20 corresponds to the region Q. Although this method is twice less effective than Gauschi-Poppe-Wijers method, nevertheless it can be used for calculating $w(z)$ with more high accuracy. Obviously, that a decrease of the grid size will lead to a reduction of the expansion (5) and, consequently, for a given accuracy of calculations will improve the speed of calculations.

The some disadvantage of this algorithm is fact that somewhat array of storage must be provided to hold the values of function $w(z)$ at the knots of the grid. However, the preservation of a two-dimensional array, even large enough, is not a big problem in the time of rapid progress in technology of information storage.

3. **Performance characteristics and tests**

Fortunately, this approach can be utilized for estimation of the maximum possible efficiency to compute this function. Really, if one reduces the step of grid a, the series (7) will converge faster and therefore the number of terms of the series can also be reduced. This process can continue until the series (7) will consist of only say four members that corresponds to the value $a = 2.5 \cdot 10^{-4}$. Calculations show that for the grid of this size the speed of calculations will be near seven times greater than the calculation using the algorithm 380. Note however, that in this case array of storage about 4GB must be provided to hold the values of function at the knots of the grid.

Conclusions

1. The extreme speed for evaluation of the complex error function in the region R is of order 1.3-1.5 times for computation of the single exponential function.
2. The speed of the complex error function evaluation can be provided twice faster than by means of the algorithm 380 with the usage of additional memory about 15KB.

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