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A rational approximation of the Dawson's integral for efficient computation of the complex error function

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ABSTRACT

In this work we show a rational approximation of the Dawson's integral that can be implemented for high accuracy computation of the complex error function in a rapid algorithm. Specifically, this approach provides accuracy exceeding $\sim 10^{-14}$ in the domain of practical importance $0 \le y < 0.1 \cap |x + iy| \le 8$. A Matlab code for computation of the complex error function with entire coverage of the complex plane is presented.

1. Introduction

The complex error function also widely known as the Faddeeva function can be defined as [1–6]

$$w(z) = e^{-z^2}\left(1 + \frac{2i}{\sqrt{\pi}}\int_0^z e^{t^2}dt\right), \tag{1}$$

where $z = x + iy$ is the complex argument. It is a solution of the following differential equation [5]

$$w'(z) + 2zw(z) = \frac{2i}{\sqrt{\pi}},$$

where the initial condition is given by $w(0) = 1$.

The complex error function is a principal in a family of special functions. The main functions from this family are the Dawson's integral, the complex probability function, the error function, the Fresnel integral and the normal distribution function.

The Dawson's integral is defined as [7–12]

$$\mathrm{daw}(z) = e^{-z^2}\int_0^z e^{t^2}dt. \tag{2}$$

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It is not difficult to obtain a relation between the complex error function and the Dawson's integral. In particular, comparing right sides of Eqs. (1) and (2) immediately yields

$$w(z) = e^{-z^2} + \frac{2i}{\sqrt{\pi}}\mathrm{daw}(z). \tag{3}$$

Another closely related function is the complex probability function. In order to emphasize the continuity of the complex probability function at $\forall y \in \mathbb{R}$, it may be convenient to define it in form of principal value integral [4–6]

$$W(z) = PV\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}dt \tag{4}$$

or

$$W(x,y) = PV\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{(x+iy)-t}dt.$$

The complex probability function has no discontinuity at $y = 0$ and $x = t$ since according to the principal value we can write

$$\lim W(x, y \to 0) = e^{-x^2} + \frac{2i}{\sqrt{\pi}}\mathrm{daw}(x), \tag{5}$$

where $x = \mathrm{Re}[z]$.

There is a direct relationship between the complex error function (1) and the complex probability function (4). In particular, it can be shown that these functions are actually same on the upper half of the complex plain [4,5]

$$W(z) = w(z), \qquad \mathrm{Im}[z] \ge 0. \tag{6}$$

Separating the real and imaginary parts of the complex probability function (4) leads to

$$K(x,y) = PV\frac{y}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{y^2+(x-t)^2}dt,$$

and

$$L(x,y) = PV\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}(x-t)}{y^2+(x-t)^2}dt, \tag{7}$$

respectively, where the principal value notations emphasize that these functions have no discontinuity at $y = 0$ and $x = t$. In particular, in accordance with Eq. (3), we can write

$$K(x, y=0) \equiv \lim K(x, y \to 0) = e^{-x^2}$$

and

$$L(x, y=0) \equiv \lim L(x, y \to 0) = \frac{2}{\sqrt{\pi}}\,\mathrm{daw}(x).$$

As it follows from the identity (6), for non-negative y we have

$$w(x,y) = K(x,y) + iL(x,y), \qquad y \ge 0. \tag{8}$$

The real part $K(x, y)$ of the complex probability function is commonly known as the Voigt function that is widely used in many disciplines of Applied Mathematics [13–15], Physics [4,16–22], Astronomy [23] and Information Technology [24]. Mathematically, the Voigt function $K(x, y)$ represents a convolution integral of the Gaussian and Cauchy distributions [5,16,17]. The Voigt function is widely used in spectroscopy as it describes quite accurately the line broadening effects [4,18–22,25].

Although the imaginary part $L(x, y)$ of the complex probability function also finds many practical applications (see for example [26,27]), it has no a specific name. Therefore, further we will regard this function simply as the L-function.

Other associated functions are the error function of complex argument [3,5]

$$\mathrm{erf}(z) = 1 - e^{-z^2}w(iz),$$