A New Application Methodology of the Fourier Transform for Rational Approximation of the Complex Error Function

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Abstract

This paper presents a new approach in application of the Fourier transform to the complex error function resulting in an efficient rational approximation. Specifically, the computational test shows that with only 17 summation terms the obtained rational approximation of the complex error function provides the average accuracy 10^{-15} over the most domain of practical importance $0 \leq x \leq 40,000$ and $10^{-4} \leq y \leq 10^2$ required for the HITRAN-based spectroscopic applications. Since the rational approximation does not contain trigonometric or exponential functions dependent upon the input parameters x and y, it is rapid in computation. Such an example demonstrates that the considered methodology of the Fourier transform may be advantageous in practical applications.

Keywords: Fourier transform, complex error function, Faddeeva function, rational approximation

1. Introduction

The forward and inverse Fourier transforms can be defined as (Bracewell, 2000; Hansen, 2014)

$$F(v) = \mathcal{F}\{f(t)\}(v) = \int_{-\infty}^{\infty} f(t)\, e^{-2\pi i v t} dt \tag{1a}$$

and

$$f(t) = \mathcal{F}^{-1}\{F(v)\}(t) = \int_{-\infty}^{\infty} F(v)\, e^{2\pi i v t} dv, \tag{1b}$$

respectfully. Approximation theory based on the Fourier trigonometric series for functions or signals remains a topical subject in mathematical analysis and many new efficient methodologies have been reported in the recent scientific literature (see for example Mishra & Mishra, 2012; Mishra *et al.* 2013; Boyd, 2013).

In our recent publication (Abrarov & Quine, 2015d) we have shown that a sampling with the Gaussian function of the kind $he^{-(t/c)^2}/\left(c\sqrt{\pi}\right)$ leads to the trigonometric approximations for the forward

$$F(v) = \mathcal{F}\{f(t)\}(v) \approx he^{-(\pi c v)^2} \sum_{n=-N}^{N} f(nh)\, e^{-2\pi i v n h} \tag{2a}$$

and inverse Fourier transforms

$$f(t) = \mathcal{F}^{-1}\{F(v)\}(t) \approx he^{-(\pi c t)^2} \sum_{n=-N}^{N} F(nh)\, e^{2\pi i t n h}, \tag{2b}$$

where h is the step between two adjacent sampling points and c is the fitting parameter, $e^{-2\pi i v n h} = \cos(2\pi i v n h) - i\sin(2\pi i v n h)$ and $e^{2\pi i t n h} = \cos(2\pi i t n h) + i\sin(2\pi i t n h)$. The parameters h, c and N in the equations (2a) and (2b) may be the same in the forward and inverse Fourier transforms only when we imply the most favorable conditions $h << 1$, $c << 1$ and $N >> 1$. In practical tasks, however, these conditions may be compromised in order to reduce the number of

the summation terms. As a result, these parameters may not be necessarily equal to each other in the forward and inverse Fourier transforms. Consequently, it is convenient to rewrite two equations above in form

$$F(v) = \mathcal{F}\{f(t)\}(v) \approx h_f e^{-(\pi c_f v)^2} \sum_{m=-M}^{M} f(mh_f) e^{-2\pi i v m h_f}$$

and

$$f(t) = \mathcal{F}^{-1}\{F(v)\}(t) \approx h_i e^{-(\pi c_i t)^2} \sum_{n=-N}^{N} F(nh_i) e^{2\pi i t n h_i},$$

where h_f, c_f, M and h_i, c_i, N are the steps, the fitting parameters and the integers corresponding to the forward and inverse Fourier transforms, respectively.

The presence of the damping functions $e^{-(\pi c_f v)^2}$ and $e^{-(\pi c_i t)^2}$ in the equations above excludes periodicity of the approximated functions $f(t)$ and $F(v)$. Consequently, a solitary wavelet (or non-periodic pulse) can be effectively approximated in the Fourier transform. However, when we take $c_f = c_i = 0$, the right side of these equations become periodic with corresponding periods $1/h_f$, $1/h_i$ and represent the Fourier-type expansion series as follows

$$F(v) \approx h_f \sum_{m=-M}^{M} f(mh_f) e^{-2\pi i v m h_f}, \qquad -\frac{1}{2h_f} \leq v \leq \frac{1}{2h_f}, \tag{3a}$$

and

$$f(t) \approx h_i \sum_{n=-N}^{N} F(nh_i) e^{2\pi i t n h_i}, \qquad -\frac{1}{2h_i} \leq t \leq \frac{1}{2h_i}. \tag{3b}$$

It should be noted that if the integral (1a) is not analytically integrable, then the function $f(t)$ can be approximated by substituting equation (3a) into (3b). This substitution yields

$$f(t) \approx h_i \sum_{n=-N}^{N} \underbrace{\left[h_f \sum_{m=-M}^{M} f(mh_f) e^{-2\pi i n h_i m h_f} \right]}_{\approx F(nh_i)} e^{2\pi i t n h_i}$$

$$= h_i h_f \sum_{n=-N}^{N} \sum_{m=-M}^{M} f(mh_f) e^{2\pi i n h_i (t - m h_f)}, \qquad -\frac{1}{2h_i} \leq t \leq \frac{1}{2h_i}.$$

In this work we show a new application methodology of the Fourier transform to the complex error function. Due to representation of the complex error function as a rational approximation, it is rapid in computation. Furthermore, with only 17 summation terms the obtained rational approximation of the complex error function provides accuracy 10^{-15} over the most domain of practical importance $0 \leq x \leq 40,000 \cap 10^{-4} \leq y \leq 10^2$ required for applications utilizing the HITRAN molecular spectroscopic database (Rothman *et al.*, 2013).

2. Derivation

2.1 Function Overview

The complex error function, also known as the Faddeeva function or the Kramp function, can be defined as (Faddeyeva & Terent'ev, 1961; Gautschi, 1970; Abramowitz & Stegun, 1972; Armstrong & Nicholls, 1972; Schreier, 1992)

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

where $z = x + iy$ is the complex argument. The complex error function is a solution of the differential equation (Schreier, 1992)

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

with initial condition $w(0) = 1$.

The complex error function is closely related to a family of the special functions. Among them the most important one is the complex probability function (Armstrong & Nicholls, 1972; Schreier, 1992; Weideman, 1994)

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

or

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

This principal value integral implies that the complex probability function has no discontinuity at $y = 0$ and $x = t$. In particular,

$$\lim W(x, y \to 0) = e^{-x^2} + \frac{2i}{\sqrt{\pi}} \text{daw}(x), \tag{4}$$

where daw (x) is the Dawson's integral that will be briefly introduced later. There is a direct relationship between complex error function and complex probability function (Armstrong & Nicholls, 1972; Schreier, 1992)

$$W(z) = w(z), \qquad \text{Im}[z] \geq 0. \tag{5}$$

The real part of the complex probability function, denoted as $K(x, y)$, is known as the Voigt function. Mathematically, the Voigt function represents a convolution integral of the Gaussian and Lorentzian distributions (Armstrong & Nicholls, 1972; Schreier, 1992; Letchworth & Benner, 2007; Pagnini & Mainardi, 2010; Abrarov $et\ al.$, 2010)

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

where the principal value integral also implies that it has no discontinuity at $y = 0$ and $x = t$. Specifically, from equation (4) it follows that

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

At non-negative argument y the real part of the complex error function is also the Voigt function in accordance with identity (5). The Voigt function is widely used in many spectroscopic applications as it describes the line broadening effects (Edwards, 1992; Quine & Drummond, 2002; Christensen $et\ al.$, 2012; Berk, 2013; Quine & Abrarov, 2013). Therefore, the application of the complex error function is very significant in quantitative spectroscopy.

Other closely related functions are the error function of complex argument (Schreier, 1992)

$$w(z) = e^{-z^2} \text{erfc}(-iz) = e^{-z^2} [1 - \text{erf}(-iz)] \quad \Leftrightarrow \quad \text{erf}(z) = 1 - e^{-z^2} w(iz),$$

the plasma dispersion function (Fried & Conte, 1961)

$$Z(z) = PV \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{t - z} dt = i\sqrt{\pi} w(z)$$

the Dawson's integral (Cody, 1970; McCabe, 1974; Rybicki, 1989; Boyd, 2008; Abrarov & Quine, 2015c)

$$\text{daw}(z) = e^{-z^2} \int_0^z e^{t^2} dt = \sqrt{\pi} \frac{-e^{-z^2} + w(z)}{2i},$$

the Fresnel integral (Abramowitz & Stegun, 1972; McKenna, 1984)

$$F_r(z) = \int_0^z e^{i(\pi/2)t^2} dt$$

$$= (1 + i) \left[1 - e^{i(\pi/2)z^2} w \left(\sqrt{\pi}(1 + i)z/2 \right) \right] / 2$$

and the normal distribution function (Weisstein, 2003)

$$\Phi(z) = \frac{1}{\sqrt{2\pi}} \int_0^z e^{-t^2/2} dt = \frac{1}{2} \text{erf} \left(\frac{z}{\sqrt{2}} \right)$$

$$= \frac{1}{2} \left[1 - e^{-z^2/2} w \left(\frac{iz}{\sqrt{2}} \right) \right].$$

It is not difficult to show that the complex error function can be represented in an alternative form (see equation (3) in (Srivastava & Miller, 1987) and (Srivastava & Chen, 1992), see also Appendix A in (Abrarov & Quine, 2015c) for derivation)

$$w(x, y) = \frac{1}{\sqrt{\pi}} \int_0^\infty \exp\left(-t^2/4\right) \exp\left(-yt\right) \exp\left(ixt\right) dt. \tag{6}$$

This representation of the complex error function will be used for derivation of a rational approximation.

2.2 Rational Approximation

In our recent publications we have shown a new technique to obtain a rational approximation for the integrals of kind (Abrarov & Quine, 2014; Abrarov & Quine, 2015b)

$$\int_0^\infty e^{-t^2} f(t) \, dt.$$

We apply this approach together with the Fourier transform methodology discussed above in the Introduction.

We can use either of equation (3a) or (3b). For example, we may choose the equation (3b) corresponding to the inverse Fourier transform. Consider the function $f(t) = e^{-t^2/4}$. Let us find first its forward Fourier transform by substituting $f(t) = e^{-t^2/4}$ into equation (1a). These leads to

$$F(v) = \int_{-\infty}^\infty e^{-t^2/4} e^{-2\pi i v t} dt = 2\sqrt{\pi} e^{-(2\pi v)^2}.$$

Now substituting $2\sqrt{\pi} e^{-(2\pi v)^2}$ into equation (3b) yields the following approximation for the exponential function

$$e^{-t^2/4} \approx 2\sqrt{\pi} h_i \sum_{n=-N}^{N} e^{-(2\pi n h_i)^2} e^{2\pi i t n h_i}, \qquad -\frac{1}{2h_i} \le t \le \frac{1}{2h_i},$$

or

$$e^{-t^2/4} \approx 2\sqrt{\pi} h_i \sum_{n=-N}^{N} e^{-(2\pi n h_i)^2} \cos\left(2\pi t n h_i\right), \qquad -\frac{1}{2h_i} \le t \le \frac{1}{2h_i}. \tag{7}$$

Taking into account that

$$e^{-(2\pi 0 h_i)^2} \cos\left(2\pi t 0 h_i\right) = 1$$

and

$$\sum_{n=-N}^{-1} e^{-(2\pi n h_i)^2} \cos\left(2\pi t n h_i\right) = \sum_{n=1}^{N} e^{-(2\pi n h_i)^2} \cos\left(2\pi t n h_i\right)$$

the approximation (7) can be simplified as given by

$$e^{-t^2/4} \approx 2\sqrt{\pi} h_i \left[1 + 2\sum_{n=1}^{N} e^{-(2\pi n h_i)^2} \cos\left(2\pi t n h_i\right)\right], \qquad -\frac{1}{2h_i} \le t \le \frac{1}{2h_i}. \tag{8}$$

The right side limitation $t \le 1/(2h_i)$ along the positive t-axis in equation (8) can be readily excluded by multiplying both its sides to $\exp(-\sigma t)$ if a constant σ is positive and sufficiently large. This can be explained by considering Fig. 1 that shows two functions computed according to right side of equation (8) at $\sigma = 0.1$ (blue curve) and $\sigma = 0.2$ (red curve). For example, at $\sigma = 0.1$ we can observe two additional peaks at $1/h_i$ and $2/h_i$ (blue curve). However, as σ increases the additional peaks are suppressed stronger to zero due to multiplication to the damping exponential function $\exp(-\sigma t)$. As a result, at $\sigma = 0.2$ only a single additional peak at $1/h_i$ remains visible (red curve). By $\sigma \gtrsim 1$ all additional peaks completely vanish and, therefore, do not contribute to error in integration. Consequently, if the constant σ is large enough, say approximately equal or greater than 1, we can write the approximation

$$e^{-t^2/4} e^{-\sigma t} \approx 2\sqrt{\pi} h_i \left[1 + 2\sum_{n=1}^{N} e^{-(2\pi n h_i)^2} \cos\left(2\pi t n h_i\right)\right] e^{-\sigma t}, \qquad \sigma \gtrsim 1,$$
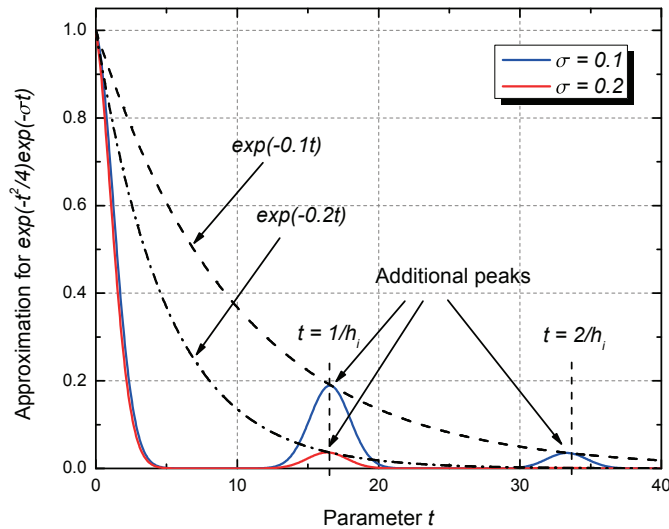
Figure 1. Function approximation for $e^{-t^2/4}e^{-\sigma t}$ at $\sigma = 0.1$ (blue curve) and $\sigma = 0.2$ (red curve). The dashed and dot-dashed curves are the exponential functions $e^{-0.1t}$ and $e^{-0.2t}$, respectively.

that remains always valid without any limitation along the positive t-axis. Assuming $y \geq 0$ we, therefore, can write now

$$e^{-t^2/4}e^{-(y+\sigma)t} \approx 2\sqrt{\pi}h_i\left[1 + 2\sum_{n=1}^{N}e^{-(2\pi nh_i)^2}\cos\left(2\pi tnh_i\right)\right]e^{-(y+\sigma)t}, \qquad \sigma \gtrsim 1. \qquad (9)$$

Since $e^{-t^2/4}e^{-yt} = e^{\sigma^2}e^{-(t-2\sigma)^2/4}e^{-(y+\sigma)t}$ from approximation (9) we obtain

$$e^{-t^2/4}e^{-yt} \approx 2\sqrt{\pi}h_i e^{\sigma^2}\left[1 + 2\sum_{n=1}^{N}e^{-(2\pi nh_i)^2}\cos\left(2\pi nh_i\left(t - 2\sigma\right)\right)\right]e^{-(y+\sigma)t}, \quad \sigma \gtrsim 1. \qquad (10)$$

Once again, due to presence of the rapidly damping exponential multiplier $e^{-(y+\sigma)t}$ this approximation is valid without any limitation along the positive t-axis. As the peak of the function $e^{-(t-2\sigma)^2/4}$ is shifted towards right with respect to the origin, we may regard to the value σ as the shift constant.

Finally, substituting approximation (10) into integral (6) yields

$$w\left(z\right) \approx i\frac{2h_i e^{\sigma^2}}{z + i\sigma} + \sum_{n=1}^{N}\frac{A_n - i\left(z + i\sigma\right)B_n}{C_n^2 - \left(z + i\sigma\right)^2}, \qquad (11)$$

where

$$A_n = 8\pi h_i^2 n e^{\sigma^2 - (2\pi h_i n)^2}\sin\left(4\pi h_i n\sigma\right),$$
$$B_n = 4h_i e^{\sigma^2 - (2\pi h_i n)^2}\cos\left(4\pi h_i n\sigma\right)$$

and

$$C_n = 2\pi h_i n.$$

As the expansion coefficients A_n, B_n and C_n are independent of the argument z, the obtained equation (11) is a rational approximation.

In algorithmic implementation it is more convenient to use ψ-function defined as

$$\psi\left(z\right) = i\frac{2h_i e^{\sigma^2}}{z} + \sum_{n=1}^{N}\frac{A_n - izB_n}{C_n^2 - z^2} \qquad (12)$$
$$\Rightarrow w\left(z\right) \approx \psi\left(z + i\sigma\right).$$

2.3 Computational Procedure and Error Analysis

Due to a remarkable property of the complex error function (McKenna, 1984; Zaghloul & Ali, 2011)

$$w(-z) = 2e^{-z^2} - w(z),$$ (13)

it is sufficient to consider only I and II quadrants in order to cover the entire complex plane. This can be seen explicitly by representation of the identity (13) in form

$$w(\pm x, -|y|) = 2e^{-(\mp x + i|y|)^2} - w(\mp x, +|y|).$$

Thus, if the parameter y is negative we can simply take it by absolute value and then compute the complex error function according to right side of this equation. Therefore, further we will always assume that $y \geq 0$.

When the argument z is large enough by absolute value, say $|x + iy| \gtrsim 15$, we can truncate the Laplace continued fraction (Gautschi, 1970; Jones & Thron, 1988)

$$w(z) = \frac{\mu_0}{z-} \frac{1/2}{z-} \frac{1}{z-} \frac{3/2}{z-} \frac{2}{z-} \frac{5/2}{z-} \frac{3}{z-} \frac{7/2}{z-} \cdots, \quad \mu_0 = i/\pi.$$

Approximation based on the Laplace continued fraction is rapid in computation. However, its accuracy deteriorates as the argument z decreases by absolute value.
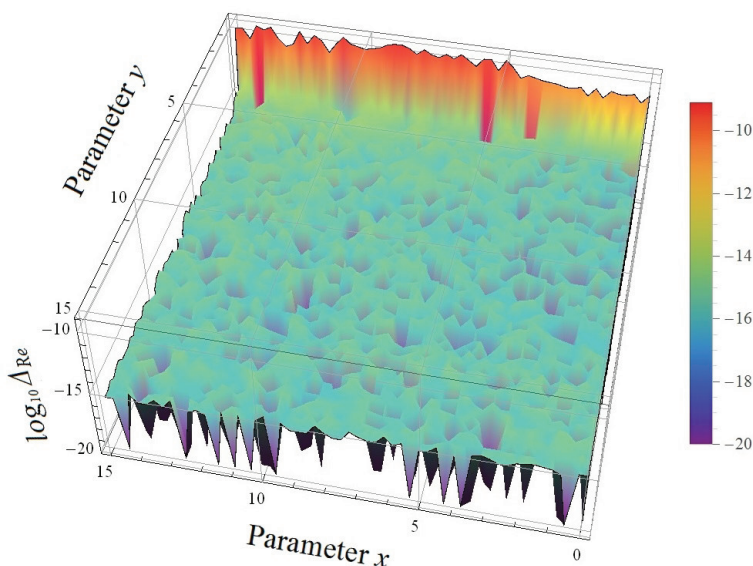

Figure 2. The logarithm of the relative error $\log_{10}\Delta_{\mathrm{Re}}$ for the real part of the rational approximation (12) over the domain $0 \leq x \leq 15 \cap 10^{-6} \leq y \leq 10^4$.

There are different approximations for computation of the narrow-band domain $0 \leq x \leq 15$ and $0 \leq y < 10^{-6}$ (Abrarov & Quine, 2014; Amamou, 2013; Abrarov & Quine, 2015a). We can apply, for example, an approximation proposed in our recent work (Abrarov & Quine, 2014)

$$w(x, y << 1) \approx \left(1 - \frac{y}{y_{\min}}\right)e^{-x^2} + \frac{y}{y_{\min}}K(x, y_{\min}) + iL(x, y_{\min}), \qquad y_{\min} << 1,$$

where $L(x, y_{\min}) = \mathrm{Im}\left[w(x, y_{\min})\right]$ and $y_{\min}$ can be taken equal to 10^{-5}. It has been shown that this approximation can provide accuracy better than 10^{-9} over the narrow-band domain $0 \leq x \leq 15$ and $0 \leq y < 10^{-6}$.

The domain $|x + iy| \leq 15 \cap y \geq 10^{-6}$ is the most difficult for computation. Nevertheless, with only 17 summation terms (at $N = 16$) the proposed rational approximation (12) covers this domain providing high-accuracy and rapid computation. In computational procedure we have to choose properly the margin value ν_m for the exponential function $e^{-(2\pi\nu)^2}$ that appears from the forward Fourier transform $F(\nu) = 2\sqrt{\pi}e^{-(2\pi\nu)^2}$. As it has been justified by Melone *et al.* 1988, the margin value

for integration involving the exponential function e^{-t^2} can be taken as $t = t_m = 6$. We can use this result in order to determine the required value by solving the following equation with respect to the variable ν as follows

$$e^{-(2\pi\nu)^2} = e^{-t^2}\Big|_{t=6} \Rightarrow (2\pi\nu)^2 = 36.$$

There are two solutions for this equation $\nu_{1,2} = \pm 6/(2\pi)$. Consequently, the margin value for the exponential function $e^{-(2\pi\nu)^2}$ can be taken as $\nu_m = 6/(2\pi)$. As a parameter h_i is the step between two adjacent sampling points along positive ν-axis (see (Abrarov & Quine 2015d) for details), its value can be calculated as $h_i = \nu_m/N$. Taking $N = 16$ we can find that $h_i = \nu_m/16 \approx 5.968310365946075 \times 10^{-2}$.

In order to quantify the accuracy of the rational approximation (12) we may define the relative errors

$$\Delta_{\text{Re}} = \left|\frac{\text{Re}\left[w_{ref}(x,y)\right] - \text{Re}\left[w(x,y)\right]}{\text{Re}\left[w_{ref}(x,y)\right]}\right|$$

and

$$\Delta_{\text{Im}} = \left|\frac{\text{Im}\left[w_{ref}(x,y)\right] - \text{Im}\left[w(x,y)\right]}{\text{Im}\left[w_{ref}(x,y)\right]}\right|,$$

where $w_{ref}(x,y)$ is the reference, for the real and imaginary parts, respectively. The highly accurate reference values can be generated by using, for example, Algorithm 680 (Poppe & Wijers, 1990a; Poppe & Wijers, 1990b), recently published Algorithm 916 (Zaghloul & Ali, 2011) or C++ code from the RooFit package, CERN's library (Karbach et al., 2014).

Figure 2 shows $\log_{10}\Delta_{\text{Re}}$ for the real part of the complex error function computed over the domain $0 \le x \le 15$ and $10^{-6} \le y \le 15$ at $N = 16$, $\sigma = 1.5$ and $h_i = 5.968310365946075 \times 10^{-2}$. As we can see from this figure, the rational approximation (12) provides accuracy 10^{-15} (blue color) over the most of this domain. Although accuracy deteriorates with decreasing y, it remains better than 10^{-9} (red color) in the range $10^{-4} \le y \le 10^{-6}$. This indicates that at the same $N = 16$ the accuracy of the rational approximation (12) is by several orders of the magnitude higher than the accuracy of the Weideman's rational approximation (see equation 38(I) in Weideman, 1994).
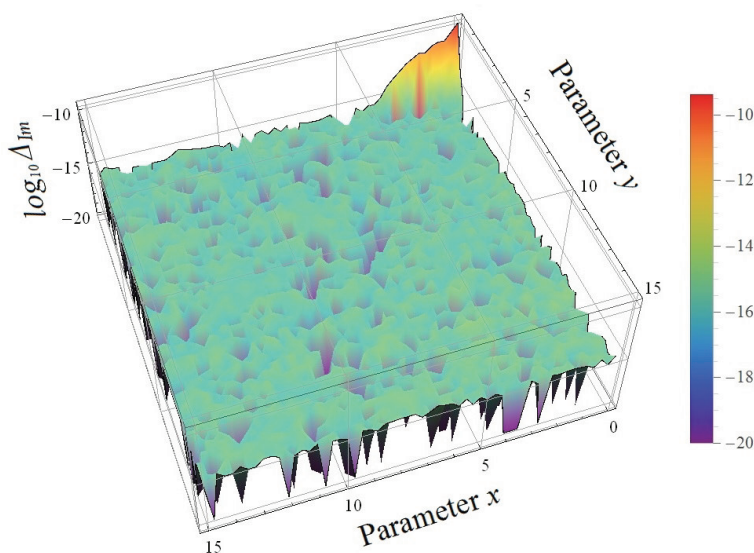

Figure 3. The logarithm of the relative error $\log_{10}\Delta_{\text{Im}}$ for the imaginary part of the rational approximation (12) over the domain $0 \le x \le 15 \cap 10^{-6} \le y \le 10^4$.

Figure 3 illustrates $\log_{10}\Delta_{\text{Im}}$ for the imaginary part of the complex error function also computed over the domain $0 \le x \le 15$ and $10^{-6} \le y \le 15$ at $N = 16$, $\sigma = 1.5$ and $h_i = 5.968310365946075 \times 10^{-2}$. One can see that in the imaginary part the accuracy is also highly accurate 10^{-15} (blue color) over the most domain. There is only a small area $0 \le x < 1$ and $10^{-6} \le y \le 10^{-4}$ near the origin where the accuracy deteriorates as the parameters x and y both tend to zero. Nevertheless, the accuracy in this area still remains high and better than 10^{-9} (red color).

The computational test reveals that with only 17 summation terms (at $N = 16$) the rational approximation (12) alone can cover the entire HITRAN domain $0 \leq x \leq 40,000 \cap 10^{-4} \leq y \leq 10^2$ providing average accuracy 10^{-15} for an input array consisting of 3×10^7 elements. Algorithmic implementation of the rational approximation (12) results to the same computational speed as that of described in our recent work where we proposed a sampling by incomplete cosine expansion of the sinc function to approximate the complex error function (Abrarov & Quine, 2015b).

A Matlab subroutine code that covers the HITRAN domain with high-accuracy is presented in Appendix A.

3. Conclusion

We present a new efficient rational approximation to the complex error function by application of the Fourier transform that provides computationally rapid and highly accurate results. The computational test we performed with only 17 summation terms shows that the accuracy of the rational approximation of the complex error function is 10^{-15} over the most domain of practical importance. In particular, the proposed rational approximation of the complex error function alone can cover with high accuracy the entire domain $0 \leq x \leq 40,000 \cap 10^{-4} \leq y \leq 10^2$ required for the HITRAN-based spectroscopic applications.

Acknowledgments

Appendix A

```
function VF = comperf(z)

% This subroutine function file computes the complex error function, also
% known as the Faddeeva function. It covers the entire HITRAN domain
% 0 <= x <= 40,000 and 10^-4 <= y <= 10^2. However, it may be used only in
% the most difficult domain |x + 1i*y| <= 15 and y > = 10^-6. See the
% article that describes how the entire complex plain can be covered.

% The code is written by Sanjar M. Abrarov and Brendan M. Quine, York
% University, October, 2015.

if any(imag(z) < 10^-6)
    disp('One or more imag(z) is less than 10^-6. Computation terminated.')
    VF = NaN;
    return
end

num = 16; % number of summation terms is 16 + 1 = 17
vm = 6/(2*pi); % margin value
hi = vm/num; % sampling step
sig = 1.5; % the shift constant

n = 1:num; % define array n

% Define the expansion coefficients
An = 8*pi*hi^2*n.*exp(sig^2 - (2*pi*hi*n).^2).*sin(4*pi*hi*n*sig);
Bn = 4*hi*exp(sig^2 - (2*pi*hi*n).^2).*cos(4*pi*hi*n*sig);
Cn = 2*pi*hi*n;

z = z + 1i*sig; % redefine input z (see formula (12) for the psi-function)
zz = z.^2;

    VF = 1i*(2*hi*exp(sig^2))./z; % define first term
    for n = 1:num
        VF = VF + (An(n) - 1i*z*Bn(n))./(Cn(n)^2 - zz);
    end
end
```

References

Abramowitz, M. & Stegun, I. A. (1972). *Error function and Fresnel integrals*. Handbook of mathematical functions with formulas, graphs, and mathematical tables. 9th Ed. Dover, New York, 297-309.

Abrarov, S. M., Quine, B. M. & Jagpal, R. K. (2010). High-accuracy approximation of the complex probability function by Fourier expansion of exponential multiplier. *Comp. Phys. Commun., 181*(5), 876-882. http://dx.doi.org/10.1016/j.cpc.2009.12.024

Abrarov, S. M. & Quine, B. M. (2014). Master-slave algorithm for highly accurate and rapid computation of the Voigt/complex error function. *J. Math. Research, 6*(2), 104-119. http://dx.doi.org/10.5539/jmr.v6n2p104

Abrarov, S. M. & Quine, B. M. (2015a). Accurate approximations of the complex error function at small imaginary argument. *J. Math. Research, 7*(1) 44-53. http://dx.doi.org/10.5539/jmr.v1n1p44

Abrarov, S. M. & Quine, B. M. (2015b). Sampling by incomplete cosine expansion of the sinc function: Application to the Voigt/complex error function. *Appl. Math. Comput. 258*, 425-435. http://dx.doi.org/10.1016/j.amc.2015.01.072

Abrarov, S. M. & Quine, B. M. (2015c). A rational approximation for the Dawson's integral of real argument, arXiv:1505.04683. http://arxiv.org/pdf/1505.04683v1.pdf

Abrarov, S. M. & Quine, B. M. (2015d). Representation of the Fourier transform as a weighted sum of the complex error functions, arXiv:1507.01241v3. http://arxiv.org/pdf/1507.01241v3.pdf

Amamou, H., Ferhat, B. & Bois, A. (2013). Calculation of the Voigt Function in the region of very small values of the parameter *a* where the calculation is notoriously difficult. *Amer. J. Anal. Chem., 4*, 725-731. http://dx.doi.org/10.4236/ajac.2013.412087

Armstrong, B. H. & Nicholls, B. W. (1972). *Emission, absorption and transfer of radiation in heated atmospheres*. Pergamon Press, New York.

Bracewell, R. N. (2000). *The Fourier transform and its application*. 3rd Ed., McGraw-Hill.

Berk, A. (2013). Voigt equivalent widths and spectral-bin single-line transmittances: Exact expansions and the MOD-TRAN ® 5 implementation. *J. Quantit. Spectrosc. Radiat. Transfer, 118*, 102-120. http://dx.doi.org/10.1016/j.jqsrt.2012.11.026

Boyd, J. P. (2008). Evaluating of Dawson's integral by solving its differential equation using orthogonal rational Cheby-shev functions, *Appl. Math. Comput., 204*(2) 914-919. http://dx.doi.org/10.1016/j.amc.2008.07.039

Boyd, J. P. (2013). A comparison of companion matrix methods to find roots of a trigonometric polynomial, *J. Comp. Phys., 246*, 96-112. http://dx.doi.org/10.1016/j.jcp.2013.03.022

Christensen, L. E., Spiers, G. D., Menzies, R. T. & Jacob, J. C. (2012) Tunable laser spectroscopy of CO_2 near 2.05 μm: Atmospheric retrieval biases due to neglecting line-mixing. *J. Quantit. Spectrosc. Radiat. Transfer, 113*(10), 739-748. http://dx.doi.org/10.1016/j.jqsrt.2012.02.031

Cody, W. J., Paciorek, K. A. & Thacher, H. C. (1970). Chebyshev approximations for Dawson's integral. *Math. Comp. 24*, 171-178. http://dx.doi.org/10.1090/S0025-5718-1970-0258236-8

Edwards, D. P. (1992). *GENLN2: A general line-by-line atmospheric transmittance and radiance model*, NCAR technical note. http://dx.doi.org/10.5065/D6W37T86

Faddeyeva, V. N. & Terentev, N. M. (1961). *Tables of the probability integral for complex argument*. Pergamon Press, Oxford, 1961.

Fried, B. D. & Conte, S.D. (1961). *The plasma dispersion function*. New York: Academic Press, 1961.

Gautschi, W. (1970). Efficient computation of the complex error function. *SIAM J. Numer. Anal., 7*(1), 187-198. http://dx.doi.org/10.1137/0707012

Hansen, E. W. (2014). *Fourier transforms. Principles and applications*. John Wiley & Sons.

Jones, W. B. & Thron, W. J. (1988). Continued fractions in numerical analysis. *Appl. Num. Math., 4*(2-4), 143-230. http://dx.doi.org/10.1016/0168-9274(83)90002-8

Karbach, T. M., Raven, G. & Schiller, M. (2014). Decay time integrals in neutral meson mixing and their efficient evaluation, arXiv:1407.0748. http://arxiv.org/pdf/1407.0748v1.pdf

Letchworth, K. L. & Benner, D. C. (2007). Rapid and accurate calculation of the Voigt function. *J. Quantit. Spectrosc. Radiat. Transfer, 107*(1), 173-192. http://dx.doi.org/10.1016/j.jqsrt.2007.01.052

McCabe, J. H. (1974). A continued fraction expansion with a truncation error estimate for Dawson's integral, *Math. Comp. 28*(127), 811-816. http://dx.doi.org/10.1090/S0025-5718-1974-0371020-3

McKenna, S. J. (1984). A method of computing the complex probability function and other related functions over the whole complex plane. *Astrophys. Space Sci., 107*(1), 71-83. http://dx.doi.org/10.1007/BF00649615

Milone, A. A. E., Milone, L. A. & Bobato, G. E. (1988). Numerical evaluation of the line broadening function. *Astrophys. Space Sci., 147*(2), 229-234. http://dx.doi.org/10.1007/BF00645667

Mishra, V. N., Khan, H. H., Khan, I. A., Khatri, K. & Mishra, L. N. (2013). Trigonometric approximation of signals (functions) belonging to the $Lip\,(\xi\,(t)\,,r)$, $(r > 1)$-class by (E,q) $(q > 0)$-means of the conjugate series of its Fourier series. *Advan. Pure Math., 2013*(3), 353-358. http://dx.doi.org/10.4236/apm.2013.33050

Mishra, V. N. & Mishra, L. N. (2012). Trigonometric approximation of signals (functions) in L_p-norm. *Int. J. Contemp. Math. Sci., 7*(19), 909-918.
http://www.m-hikari.com/ijcms/ijcms-2012/17-20-2012/narayanmishraIJCMS17-20-2012.pdf

Pagnini, G. & Mainardi, F. (2010). Evolution equations for the probabilistic generalization of the Voigt profile function. *J. Comput. Appl. Math., 233*(6), 1590-1595. http://dx.doi.org/10.1016/j.cam.2008.04.040

Poppe, G. P. M. & Wijers, C. M. J. (1990a). More efficient computation of the complex error function. *ACM Transact. Math. Software, 16*(1), 38-46. http://dx.doi.org/10.1145/77626.77629

Poppe, G. P. M. & Wijers, C. M. J. (1990b). Algorithm 680: evaluation of the complex error function. *ACM Transact. Math. Software, 16*(1), 47. http://dx.doi.org/10.1145/77626.77630

Quine, B. M. & Abrarov, S. M. (2013). Application of the spectrally integrated Voigt function to line-by-line radiative transfer modelling. *J. Quantit. Spectrosc. Radiat. Transfer, 127*, 37-48.
http://dx.doi.org/10.1016/j.jqsrt.2013.04.020

Quine, B. M. & Drummond, J. R. (2002). GENSPECT: a line-by-line code with selectable interpolation error tolerance, *J. Quant. Spectrosc. Radiat. Transfer 74*(2), 147-165.
http://dx.doi.org/10.1016/S0022-4073(01)00193-5

Rothman, L. S., Gordon, I. E., Babikov, Y., Barbe, A., Benner, D. C., *et al.* (2013). The HITRAN2012 molecular spectroscopic database, *J. Quant. Spectrosc. Radiat. Transfer, 130,* 4-50.
http://dx.doi.org/10.1016/j.jqsrt.2013.07.002

Rybicki, G. B. (1989). Dawson's integral and the sampling theorem, *Comp. Phys., 3*(2), 85-87.
http://dx.doi.org/10.1063/1.4822832

Schreier, F. (1992). The Voigt and complex error function: A comparison of computational methods. *J. Quant. Spectrosc. Radiat. Transfer, 48*(5, 6), 743-762. http://dx.doi.org/10.1016/0022-4073(92)90139-U

Srivastava H. M. & Miller, E. A. (1987). A unified presentations of the Voigt functions, *Astrophys. Space Sci., 135*(1), 111-118. http://dx.doi.org/ 10.1007/BF00644466

Srivastava, H. M. & Chen, M. P. (1991). Some unified presentations of the Voigt functions. *Astrophys. Space Sci., 192*(1), 63-74. http://dx.doi.org/10.1007/BF00653260

Weideman, J. A. C. (1994). Computation of the complex error function. *SIAM J. Numer. Anal., 31*(5), 1497-1518. http://dx.doi.org/10.1137/0731077

Weisstein, E. W. (2003). *CRC concise encyclopedia of mathematics*. Chapman & Hall/CRC, 2nd Ed.

Zaghloul, M. R. & Ali, A. N. (2011). Algorithm 916: computing the Faddeyeva and Voigt functions. *ACM Transact. Math. Software, 38*(2), 15:1-15:22. http://dx.doi.org/10.1145/2049673.2049679

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