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Computation of the Complex Probability Function

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ABSTRACT

The complex probability function is important in many areas of physics and many techniques have been developed in an attempt to compute it for some z quickly and efficiently. Most prominent are the methods that use Gauss-Hermite quadrature, which uses the roots of the n^{th} degree Hermite polynomial and corresponding weights to approximate the complex probability function. This document serves as an overview and discussion of the use, shortcomings, and potential improvements on the Gauss-Hermite quadrature for the complex probability function.

INTRODUCTION

The complex probability function (CPF),

$$w(z) = e^{-z^2}\text{erfc}(-iz), \tag{1}$$

where $z = x + iy$, can be written in integral form [1],

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

as shown in Appendix Section 1. If z's imaginary component $y \geq 0$, then $w(z)$ can also be written as

$$w(z) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}\,dt \tag{3}$$

and subsequently separated into its real and imaginary parts $u(x, y)$ and $v(x, y)$ [2], respectively, as shown in Appendix Section 2. The results of Appendix Section 2 are summarized below.

$$\begin{aligned} w(x,y) &= u(x,y) + i\,v(x,y) \\ \text{where } u(x,y) &= \frac{y}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{(x-t)^2+y^2}\,dt \\ \text{and } v(x,y) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}\,(x-t)}{(x-t)^2+y^2}\,dt \end{aligned} \tag{4}$$

GAUSS-HERMITE QUADRATURE

One of the most prominent attempts to efficiently integrate the CPF for some given complex value z is by using the method of Gauss-Hermite quadrature [3]. This technique uses the roots of the n^{th} Hermite polynomial $t_i^{(n)}$ to approximate an integral of the form

$$\int_{-\infty}^{\infty} e^{-t^2} f(t)\,dt \approx \sum_{i=1}^{n} f\left(t_i^{(n)}\right) w_i \tag{5}$$

where w_i is a constant weight corresponding to some $t_i^{(n)}$. For the purposes of integrating the CPF, Gauss-Hermite quadrature can be used,

$$\int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}\,dt \approx \sum_{i=1}^{n}\frac{\omega_i}{z-t_i}. \tag{6}$$

However, notice that if $y = \text{Im}(z)$ is very small, then the integrand of Eq. 6 becomes very singular and cannot be approximated well using a polynomial-based approach like Gauss-Hermite quadrature.

Error Estimate of CPF Gauss-Hermite Quadrature

To better understand impact that a small imaginary component y value has on the reliability of Gauss-Hermite quadrature, the error is calculated in terms of y.

$$\text{Error} = \int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}\,dt - \sum_{i=1}^{n}\frac{\omega_i}{z-t_i} = \frac{n!\sqrt{\pi}}{2^n(2n)!}f^{(2n)}(\xi) \tag{7}$$

The error of Gauss-Hermite quadrature is equal to the CPF integral shown in Eq. 3 minus the Gauss-Hermite approximation, shown in Eq. 6. This difference is found to be dependent on n (the degree of Hermite polynomials used) and the $(2n)^{th}$ derivative of $f(\xi) = (z-\xi)^{-1}$ [4]. Note that in Eq. 7, ξ is unknown.

To evaluate the error, first the $(2n)^{th}$ derivative $f(\xi)$ is evaluated to be

$$f^{(2n)}(\xi) = (2n)!(z-\xi)^{-(2n+1)}, \tag{8}$$

which is then used to simplify Eq. 7 as shown below.

$$\text{Error} = \frac{n!\sqrt{\pi}}{2^n(2n)!}f^{(2n)}(\xi) = \frac{n!\sqrt{\pi}}{2^n(z-\xi)^{2n+1}} \tag{9}$$

To get an upper bound for the error, realize that the worst error occurs when $(z-\xi)$ is minimized, which means that z's real component x must approximately equal this arbitrary real value ξ. Thus, the worst case error occurs when $(z-\xi) = y$. Stirling's approximation $n! \leq n^{n+0.5}\,e^{-n+1}$ [5] is used to further simplify the error to

$$\text{Error} \leq \frac{n^{n+1/2}\,e^{-n+1}\sqrt{\pi}}{2^n\,y^{2n+1}}. \tag{10}$$

To better understand the behavior of this maximum error, a plot of Eq. 10 is shown in Fig. 1. Note that while the maximum error in Fig. 1 is shown to quickly increase with sufficiently large n, that does not indicate that the error itself will increase accordingly. But it does reinforce the danger of error occurrence with small y.

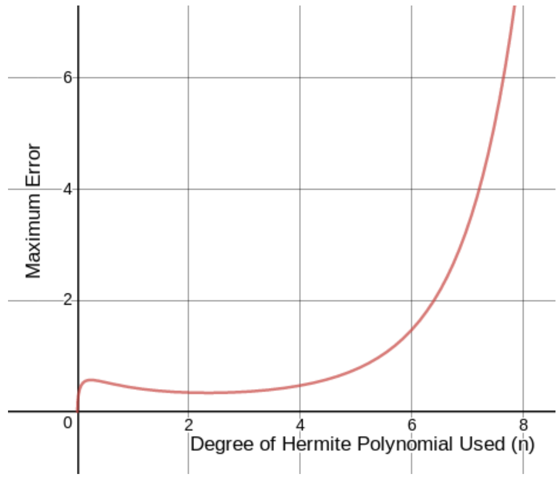

Fig. 1: Maximum error shown in Fig. 10, with n plotted along the x-axis and $y = 1.1$. Note that the maximum error begins to drastically increase for sufficiently large n.

IMPROVED GAUSS-HERMITE QUADRATURE

To account for the aforementioned shortcomings in the Gauss-Hermite quadrature approach to integrating the CPF, a number of proposed solutions have been made [1, 3, 6]. For instance, Eq. 6 can be amended to maintain a minimum positive value in its denominator, provided that z's imaginary component y is non-negative. This formulation can be seen in

$$w(z) \approx \sum_{k=1}^{n} \frac{\alpha_k^{(n)} + i\beta_k^{(n)}}{z - \gamma_k^{(n)} + i\delta_k^{(n)}} \tag{11}$$

where $\alpha_k^{(n)}$,$\beta_k^{(n)}$, $\gamma_k^{(n)}$, and $\delta_k^{(n)}$ are all real values [3]. Note that if $\delta_k^{(n)}$ is positive and z's imaginary component $y \geq 0$, then the positive offset in the denominator is maintained and the aforementioned rapid, unrepresentative spike in the summation can be avoided.

This alternative representation has restrictions however, namely to ensure that Eq. 11 reduces to Eq. 6 in the limit of large $|z|$. To do so, we require that

$$\sum_{k=1}^{n} \left(\alpha_k^{(n)} + i\beta_k^{(n)}\right) = \frac{i}{\sqrt{\pi}}(1 + \epsilon), \tag{12}$$

where ϵ is the assumed relative error of Eq. 11.

In another formulation, Eq. 6 can be replaced with another rational function,

$$w(z) \approx \frac{\sum_{k=1}^{n} a_k(-iz)^{k-1}}{(-iz)^n + \sum_{k=1}^{n} b_k(-iz)^{k-1}}, \tag{13}$$

where a_k and b_k are both real [6].

Minimization Techniques

In order for any of the aforementioned techniques (Eqs. 11,13) to be effective, a minimization technique must be used to appropriately select the constants. Selection of a certain minimization technique should account for required accuracy in the real and imaginary components of the solution (recall Eq. 4 that separates $w(z)$).

One potential option is to select the coefficients that minimize the squared error modulus on the real axis [1]. Alternatively, the coefficients may be selected such that the relative error of $w(z)$'s real component $u(0, y)$ is minimized along the imaginary half-axis (since the majority of the preceeding discussion is limited to $y \geq 0$) [3]. This is perhaps an unsatisfactory minimization technique for purposes particularly concerned about the accuracy of both the real and imaginary results ($u(x, y)$ and $v(x, y)$).

If accuracy of the imaginary component $v(x, y)$ is especially desired, then a potentially attractive option could be to minimize $v(x, 0)$ error along the real axis [1]. This could potentially lead to significant errors of the real component $u(x, y)$ near the $y = 0$ axis, and [1] suggests possible solutions.

ALTERNATIVE TO GAUSS-HERMITE QUADRATURE

Gauss-Hermite quadrature is an attractive option for solving the CPF because it makes use of the exponential in the integrand of Eq. 3 and has bounds of $(-\infty, \infty)$. That being said, an alternative to this approach is presented below, using finite integration bounds and allowing the tails of the distribution to be counted as error.

$$\int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t}\, dt = \int_{-a}^{a} \frac{e^{-t^2}}{z - t}\, dt + \int_{|t|>a} \frac{e^{-t^2}}{z - t}\, dt \tag{14}$$

So assume for instance that the integral over $[-a, a]$ in Eq. 14 can be evaluated rather well for some a. The error term, in which case, is of significant interest to determine the legitimacy and validity of this technique. Appendix Section 3 shows that the absolute value of such an error is constrained to some maximum value,

$$\left| \int_{|t|>a} \frac{e^{-t^2}}{z - t}\, dt \right| \leq \frac{1}{ya} e^{-a^2} \tag{15}$$

This maximum error illustrates that a small y value can be appropriately compensated by choosing large a. A large a value is likely feasible if $|z|$ is sufficiently large, such that the singular region does not appear in the integral from $-a$ to a.

RESTRICTION TO THE IMAGINARY HALF-AXIS

This entire discussion since Eq. 3 has been subject to the requirement that z's imaginary component y must be greater than or equal to zero. This argument can, however, be easily extended to all z values, spanning the entire complex plane [7]. Consider again Eq. 1, which defines the CPF.

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz) \tag{1}$$

This definition of $w(z)$ is shown in Appendix Section 4 to obey the following relationship:

$$w(z) = 2e^{-z^2} - w(-z) \tag{16}$$

which, when presented in terms of z's complex components, appears as

$$w(x + iy) = 2e^{-(x+iy)^2} - w(-x - iy). \quad (17)$$

Thus, if given some z with a negative imaginary component y, the sign of y can be easily flipped by using some offset dependent on z. Note that the sign of the real component x is flipped as well, but this presents no conflict since there are no constraints on the sign of x.

APPENDIX

1 - CPF Relation

$$w(z) = e^{-z^2}\mathrm{erfc}(-iza) \tag{A.1}$$

We use the standard error function identities:

$$\mathrm{erfc}(-iz) = 1 - \mathrm{erf}(-iz), \tag{A.2}$$

$$i\,\mathrm{erfi}(-z) = \mathrm{erf}(-iz), \tag{A.3}$$

$$\mathrm{erfi}(-z) = \frac{2}{\sqrt{\pi}}\int_0^{-z} e^{t^2}\,dt = -\frac{2}{\sqrt{\pi}}\int_0^{z} e^{t^2}\,dt. \tag{A.4}$$

Combining Eq. A.2, Eq. A.3, and Eq. A.4, we find that

$$\mathrm{erfc}(-iz) = 1 + \frac{2i}{\sqrt{\pi}}\int_0^{z} e^{t^2}\,dt \tag{A.5}$$

which, when used in Eq. A.1, illustrates that

$$w(z) = e^{-z^2}\left(1 + \frac{2i}{\sqrt{\pi}}\int_0^{z} e^{t^2}\,dt\right) \tag{A.6}$$

2 - $w(z)$ Real and Imaginary Parts

Recall Eq. 3, which illustrates an alternate definition of $w(z)$ subject to its imaginary component $y \geq 0$,

$$w(z) = \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t}\,dt. \tag{3}$$

$$w(x,y) = \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{x+iy-t}\,dt \tag{A.7}$$

$$w(x,y) = \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{x-t+iy} \times \frac{x-t-iy}{x-t-iy}\,dt \tag{A.8}$$

$$w(x,y) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}\,(ix-it+y)}{(x-t)^2+y^2}\,dt \tag{A.9}$$

$$w(x,y) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}\,y}{(x-t)^2+y^2}\,dt + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}\,(ix-it)}{(x-t)^2+y^2}\,dt \tag{A.10}$$

$$w(x,y) = \frac{y}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{(x-t)^2+y^2}\,dt + \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}\,(x-t)}{(x-t)^2+y^2}\,dt \tag{A.11}$$

$$w(x,y) = u(x,y) + i\,v(x,y) \tag{A.12}$$

where $u(x,y)$ is the Voigt function, which is a convolution of Gauss and Lorentzian profiles [2].

3 - Bound for tails of integral

Consider the absolute value of the error term in Eq. 14, which is never greater than the integral of its absolute value,

$$\text{Error} = \left| \int_{|t|>a} \frac{e^{-t^2}}{z-t}\,dt \right| \leq \int_{|t|>a} \frac{e^{-t^2}}{|z-t|}\,dt. \tag{A.13}$$

This can be further bounded by considering instead the maximum value of the $|z-t|^{-1}$ term,

$$\text{Error} \leq \int_{|t|>a} e^{-t^2} \max\left(\frac{1}{|z-t|}\right)\,dt. \tag{A.14}$$

Notice that the maximum value of the above fraction occurs when z and t are closest to each other. This corresponds to a situation where z's real component x is equal to t, meaning that $|z-t|$ is equal to y. Left with the integration of a symmetric function, the integration now considers only one tail.

$$\text{Error} \leq \int_{|t|>a} e^{-t^2}\frac{1}{y}\,dt = \frac{2}{y}\int_{t>a} e^{-t^2}\,dt \tag{A.15}$$

To estimate the size of this Gaussian tail, the integrand is first multiplied by t/a, which is still valid as an upper bound since $t/a \geq 1$ (all values of t considered are chosen such that $t > a$).

$$\text{Error} \leq \frac{2}{y}\int_{t>a} \frac{t}{a}e^{-t^2}\,dt = \frac{2}{ya}\int_{t>a} te^{-t^2}\,dt \tag{A.16}$$

At this point, a substitution is made where $u = t^2$ and $du = 2t\,dt$

$$\text{Error} \leq \frac{1}{ya}\int_{u>a^2} e^{-u}\,du = \frac{1}{ya}e^{-a^2} \tag{A.17}$$

4 - Relating $w(z)$ to $w(-z)$

Consider Eq. 1 for both positive and negative argument z.

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

$$w(z) = e^{-z^2}\mathrm{erfc}(-iz) \tag{A.18}$$

$$w(-z) + w(z) = e^{-z^2}\Big(\mathrm{erfc}(iz) + \mathrm{erfc}(-iz)\Big) \tag{A.19}$$

$$w(-z) + w(z) = e^{-z^2}\Big(1 - \mathrm{erf}(iz) + 1 - \mathrm{erf}(-iz)\Big) \tag{A.20}$$

$$w(-z) + w(z) = e^{-z^2}\left(2 - \frac{1}{\sqrt{\pi}}\int_{-iz}^{iz} e^{-t^2}\,dt - \frac{1}{\sqrt{\pi}}\int_{iz}^{-iz} e^{-t^2}\,dt\right) \tag{A.21}$$

$$w(-z) + w(z) = e^{-z^2}\left(2 - \frac{1}{\sqrt{\pi}}\int_{-iz}^{iz} e^{-t^2}\,dt + \frac{1}{\sqrt{\pi}}\int_{-iz}^{iz} e^{-t^2}\,dt\right) \tag{A.22}$$

$$w(-z) + w(z) = 2e^{-z^2} \tag{A.23}$$

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