Reconstruction: Rational Approximation of the Complex Error Function and the Electric Field of a Two-Dimensional Gaussian Charge Distribution

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February 14, 2023

Abstract

To simulate the beam-beam interaction one needs efficient formulae for the evolution of the electric field of a two-dimensional complex charge distribution which can be expressed in terms of the complex error function $w(z)$. This paper shows how to approximate $w(z)$ by a set of rational functions. The percent error of the approximation is extremely small. ($\sim 10^{-4}$ except near the real axis) and the electric fields are also provided.

1 Introduction

For the simulation of the beam-beam interaction one needs to evaluate the electric field of a two-dimensional Gaussian charge distribution. The electric field at the position (x, y) has been found by M. Bassetti and G.A. Erskine[1] to have the following form:[2]

$$E_x = \frac{Q}{2\epsilon_0\sqrt{2\pi(s_x^2 - s_y^2)}} \Im\left(w\Big(\frac{x+iy}{\sqrt{2(s_x^2-s_y^2)}}\Big) - e^{-\left(\frac{x^2}{2s_x^2}+\frac{y^2}{2s_y^2}\right)}\, w\Big(\frac{x\frac{s_y}{s_x}+iy\frac{s_x}{s_y}}{\sqrt{2(s_x^2-s_y^2)}}\Big)\right) \tag{1.1}$$

$$E_y = \frac{Q}{2\epsilon_0\sqrt{2\pi(s_x^2 - s_y^2)}} \Re\left(w\Big(\frac{x+iy}{\sqrt{2(s_x^2-s_y^2)}}\Big) - e^{-\left(\frac{x^2}{2s_x^2}+\frac{y^2}{2s_y^2}\right)}\, w\Big(\frac{x\frac{s_y}{s_x}+iy\frac{s_x}{s_y}}{\sqrt{2(s_x^2-s_y^2)}}\Big)\right) \tag{1.2}$$

where Q is a constant with a dimension of electric charge, ϵ_0 is the electric permittivity of free space, s_x and s_y ($s_x > s_y$ assumed) are the standard deviations of the charge distribution in the x and y directions, respectively, and $w(z)$ is the complex error function[3] defined by

$$w(z) = \int_0^{-z^2} \Big(1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{u^2}\, du\Big). \tag{1.3}$$

We shall approximate $w(z)$ by rational functions so that a computer can *quickly* handle the evaluation of $w(z)$ and thus the electric field of a two-dimensional Gaussian charge distribution. Though we were originally interested in an approximation good to within 1% error, the result turned out to be a much better approximation. We note that after the approximation of $w(z)$ the only transcendental function in (1.1) and (1.2) which spend a longer computing time than rational functions are the exponential factors. We also note that by the symmetry properties of $w(z)$[3] it suffices to approximate $w(z)$ only in the first quadrant of the complex plane.

2 Padé Approximation

We shall briefly describe how the Padé approximation is done first, then apply the approximation to the function $w(z)$.

Suppose that we have a complex-valued function $f(z)$ which is analytic at a point z_0 and suppose that we want to approximate it around z_0 by a rational function of the form

$$f_{\text{Pade}}(z) = \frac{\sum_{k=0}^{M} c_k (z - z_0)^k}{1 + \sum_{k=1}^{N} d_k (z - z_0)^k} \tag{2.1}$$

where $c_k, d_k \in \mathfrak{C}$ are unknown (possibly complex) coefficients to be determined. Note: We must have $d_0 \neq 0$ because $f(z)$ is well behaved at z_0. We may set $d_0 = 1$. For, otherwise, we can always divide both the numerator and denominator by d_0.

Here we choose M and N according to how much accuracy we need. In order to determine the coefficients c_k and d_k we impose a condition on f_{Pade}:

$$f - f_{\text{Pade}} = A_1 (z - z_0)^{M+N+1} + A_2 (z - z_0)^{M+N+2} + \cdots, \tag{2.2}$$

where $A_1, A_2, \cdots \in \mathfrak{C}$ are some constants. That is, the error introduced by the approximation at z with $|z - z_0| < 1$ is of the order of $|z - z_0|^{M+N+1}$ and very small if M and N are large. Since f is analytic at z_0 we have a Taylor series at z_0:

$$f(z) = \sum_{j=0}^{\infty} a_j (z - z_0)^j; \quad a_j \in \mathfrak{C}. \tag{2.3}$$

Then using (2.3) for f in (2.2), multiplying both sides of (2.2) by the denominator of f_{Pade}, and equating the coefficients of the powers of $(z - z_0)$ in both sides of the equation, we have the following relationships among a_k, c_k, and d_k:

$$\begin{array}{lcc} (z-z_0)^0: & c_0 = & a_0 \\ (z-z_0)^1: & c_1 - a_0 d_1 = & a_1 \\ (z-z_0)^2: & c_2 - a_1 d_1 - a_0 d_2 = & a_2 \\ (z-z_0)^3: & c_3 - a_2 d_1 - a_1 d_2 - a_0 d_3 = & a_3 \\ \quad\cdots & \cdots & \\ (z-z_0)^k: & c_k - a_{k-1} d_1 - a_{k-2} d_2 - \cdots - a_0 d_k = & a_k \end{array} \tag{2.4}$$

where $c_k = 0$ for $k > M$ and $d_k = 0$ for $k > N$. In a matrix language we have

$$\begin{pmatrix} 1 & & & & -a_0 & & & \\ & 1 & & 0 & -a_1 & -a_0 & & 0 \\ & & 1 & & -a_2 & -a_1 & -a_0 & \\ & & & \ddots & \vdots & \vdots & & \ddots \\ & & & 1 & -a_{M-1} & -a_{M-2} & \cdots & -a_{M-N} \\ & 0 & & & -a_M & -a_{M-1} & \cdots & -a_{M-N+1} \\ & & & & -a_{M+1} & -a_M & \cdots & -a_{M-N+2} \\ & & & & & & & \\ & & & & -a_{M+N-1} & -a_{M+N-2} & \cdots & -a_M \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_M \\ d_1 \\ d_2 \\ \vdots \\ d_N \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_M \\ a_{M+1} \\ a_{M+2} \\ \vdots \\ a_{M+N} \end{pmatrix} \tag{2.5}$$

where $a_k = 0$ for $k < 0$. By inverting this matrix we can determine the coefficients c_j and d_k ($j = 1, \cdots, M$ and $k = 1, \cdots, N$). Note: the inversion of this kind of matrices is easily done by computers. (Cf. IBM 360 Scientific Subroutine Package (SSP).)

2.1 PADE 1

The Taylor series of $w(z)$ around the origin is[3]

$$w(z) = \sum_{j=0}^{\infty} a_j z^j = \sum_{j=0}^{\infty} a_j z^j \, \frac{(iz)^j}{\Gamma(j/2+1)}. \tag{2.6}$$

Let

$$u = iz = -ZI + iZR, \quad \text{where } z = ZR + iZI. \tag{2.7}$$

Then

$$w(z) \overset{\text{Def.}}{=} G(u) = \sum_{j=0}^{\infty} \frac{u^j}{\Gamma(j/2+1)}. \tag{2.8}$$

We shall apply the Padé approximation to $G(u)$. Considering the behavior of $w(z)$

$$w(z) \to 0 \text{ as } |z| \to \infty$$

for those z such that $|ZR| > |ZI|$, we take

$$M = 6 \text{ and } N = 7.$$

By inverting the matrix (2.5) we obtain, up to nine significant figures,

$$\begin{array}{ll} c_0 = 1 \quad (\text{Cf. } (2.4)\,) & d_1 = -2.38485635 \\ c_1 = -1.25647718 & d_2 = 2.51608137 \\ c_2 = 8.25059158 \times 10^{-1} & d_3 = -1.52579040 \\ c_3 = -3.19300157 \times 10^{-1} & d_4 = 5.75922693 \times 10^{-1} \\ c_4 = 7.63191605 \times 10^{-2} & d_5 = -1.35740709 \times 10^{-1} \\ c_5 = -1.04697938 \times 10^{-2} & d_6 = 1.85678083 \times 10^{-2} \\ c_6 = 6.44878652 \times 10^{-4} & d_7 = -1.14243694 \times 10^{-3} \end{array} \tag{2.9}$$

Hence the approximation of $w(z)$ near the origin is, by (2.1)

$$w(z) = G(u) \approx \frac{1 + c_1 u + c_2 u^2 + c_3 u^3 + c_4 u^4 + c_5 u^5 + c_6 u^6}{1 + d_1 u + d_2 u^2 + d_3 u^3 + d_4 u^4 + d_5 u^5 + d_6 u^6 + d_7 u^7}, \tag{2.10}$$

where $u = -ZI + iZR$, and the corfficints c_k and d_k are given by (2.9).

2.2 PADE 2

Since the approximation PADE 1 behaves rather poorly along the real axis right around $z = 3$ (Cf. Table 2), we need a Padé approximation around $z = 3$. The Taylor series of $w(z)$ at $z = 3$ is

$$w(z) = \sum_{j=0}^{\infty} (z-3)^j, \tag{2.11}$$

where

$$a_j = \frac{w^{(j)}(3)}{j!}. \tag{2.12}$$

The derivatives $w^{(j)}(3)$ can be expressed in terms of $w(3)$ by use of the relations[3]

$$\begin{gathered} w^{(j+2)}(z) + 2zw^{(j+1)}(z) + 2(j+1)w^{(j)}(z) = 0, \quad (j = 0, 1, 2, \cdots) \\ w^{(0)}(z) = w(z), \quad w'(z) = -2zw(z) + \tfrac{2i}{\sqrt{\pi}}. \end{gathered} \tag{2.13}$$

On the other hand, the value of $w(3)$ is, by (1.3)

$$w(3) = e^{-9} + \frac{2i}{\sqrt{\pi}} e^{-9} \int_0^3 e^{u^2} \, du. \tag{2.14}$$

By using Table 2 in Rosser[4] for the value of the second term we have w_3 up to nine significant figures:

$$w(3) = 1.23409804 \times 10^{-4} + i2.01157318 \times 10^{-1}. \tag{2.15}$$

This time we choose

$$M = 3 \text{ and } N = 4.$$

By inverting the matrix (2.5) we obtain, up to nine significant figures,

$$\begin{aligned}
c_0 &= 1.23409804 \times 10^{-4} + i2.01157318 \times 10^{-1} \quad \text{(Cf. (2.4))}\\
c_1 &= 2.33746715 \times 10^{-1} + i1.61133338 \times 10^{-1}\\
c_2 &= 1.25689814 \times 10^{-1} - i4.04227250 \times 10^{-2}\\
c_3 &= 8.92089179 \times 10^{-3} - i1.81293213 \times 10^{-2}\\
d_1 &= 1.19230984 - i1.16495901\\
d_2 &= 8.94015450 \times 10^{-2} - i1.07372867\\
d_3 &= -1.68547429 \times 10^{-1} - i2.70096451 \times 10^{-1}\\
d_4 &= -3.20997564 \times 10^{-2} - i1.58578639 \times 10^{-2}
\end{aligned} \tag{2.16}$$

Hence the approximation of $w(z)$ near the origin is, by (2.1)

$$w(z) = G(u) \approx \frac{1 + c_1 u + c_2 u^2 + c_3 u^3}{1 + d_1 u + d_2 u^2 + d_3 u^3 + d_4 u^4}, \tag{2.17}$$

where the corfficints c_k and d_k are given by (2.16).

3 Asymptopic Expression

Away from the origin and $z = 3$ we can use the asymptotic expression for $w(z)$ given by Faddeyeva and Terent'ev, (Eqn. (10))[5]. The formula is

$$w(z) \approx \sum_{k=1}^{n} \frac{i\lambda_k^{(n)}}{\pi(z - x_k^{(n)})} = \sum_{k=1}^{n} \frac{i a_k^{(n)}}{\pi(z - x_k^{(n)})}, \quad a_k^{(n)} = \frac{\lambda_k^{(n)}}{\pi}. \tag{3.1}$$

where $x_k^{(n)}$ are the roots of Hermite polynomials and $\lambda_k^{(n)}$ are the corresponding coefficients (and n is an integer related to the accuracy of the approximation). The values of $x_k^{(n)}$ and $\lambda_k^{(n)}$ are found in Greenwood and Miller[6]. By choosing $n = 10$, we have an asymptotic approximation of $w(z)$ as

$$w(z) \approx \frac{ia_1}{z - x_1} + \frac{ia_1}{z + x_1} + \frac{ia_2}{z - x_2} + \frac{ia_2}{z + x_2} + \frac{ia_3}{z - x_3} + \frac{ia_3}{z + x_3} + \frac{ia_4}{z - x_4} + \frac{ia_4}{z + x_4} + \frac{ia_5}{z - x_5} + \frac{ia_5}{z + x_5}, \tag{3.2}$$

where the coefficients, up to nine or ten significant figures, are

$$\begin{aligned}
a_1 &= 1.94443615 \times 10^{-1} & x_1 &= 3.42901327 \times 10^{-1}\\
a_2 &= 7.64384940 \times 10^{-2} & x_2 &= 1.036610830\\
a_3 &= 1.07825546 \times 10^{-2} & x_3 &= 1.756683649\\
a_4 &= 4.27695730 \times 10^{-4} & x_4 &= 2.532731674\\
a_5 &= 2.43202531 \times 10^{-6} & x_5 &= 3.436159119
\end{aligned} \tag{3.3}$$

4 Regions of Validity of the Three Approximations

5 Boundaries of the Valid Regions of the Three Approximations

6 Electric Field

Once we have the function $w(z)$, we can find the electric field by simply using the formulae (1.1) and (1.2). We set, for simplicity,

$$\frac{Q}{2\epsilon_0\sqrt{\pi}} = 1 \tag{6.1}$$

in those formulae.

Unfortunately, there is one problem: By symmetry $E_y = 0$ for $y = 0$. But we know $\Re w(z)$ is not approximated well near the real axis, so the two terms in (1.2) might not cancel out each other to give exactly zero at $y = 0$. This might cause the percent error for E_y to be rather large for $y = 0$ and y small. To overcome this difficulty we first set $E_y = 0$ if $y = 0$ and *linearly interpolate* the values of E_y for y very small. That is, for

$$\frac{y}{\sqrt{2(s_x^2 - s_y^2)}} < 0.002,$$

we set

$$E_y = \frac{\frac{y}{\sqrt{2(s_x^2 - s_y^2)}}}{0.002} E_y(x, 0.002\sqrt{2(s_x^2 - s_y^2)}) \tag{6.2}$$

(Cf. Program 1 and Table 5.) This also serves to guarantee that $E_y(x, y)$ will be continuous between the first and fourth quadrants.

7 Concluding Remarks

The program FNCTNW calculates $w(z)$ quite accurately. The percent error in most of the region is $\sim 10^{-4}\%$ except for the real part of $w(z)$ near the real axis for certain values of ZR (near ZR = 2.2, 3.5, and 4.2) where the percent error could be at most 0.1%.

The program GAFELD likewise calculates the electric field with the percent error $\sim 10^{-4}\%$ except for E_y near the real axis where the percent error could be at most 0.1%.

Even though we have rather large percent errors (~0.1%) for $\Re w(z)$ and E_y near the real axis, the *absolute errors* are small because $\Re w(z)$ and E_y take on small absolute values there.

We have discussed the accurate evaluation over the entire first quadrant. If used in a computer simulation of beam-beam effects, PADE 1 would be called by far the most, as its region of validity more or less corresponds to where the particles reside. One may be justified, for the sake of simplicity, in regarding PADE 1 as an adequate replacement for the true field, but further investigation would be necessary to confirm this.

Acknowledgements

We would like to thank Professor W. Fuchs in Mathematics Department of Cornell University for various useful discussions.

References

[1] M. Bassetti and G.A. Erskine, *Closed expression for the electric field of a two-dimensional Gaussian charge,* CERN-ISR-TH/80-06 (unpublished)

[2] A typographical error in the formula of Bassetti and Erskine has been corrected. (The sign of the second term in the exponential factor has been reversed.)

[3] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions,* National Bureau of Standards, Washington, Chapter 7, 1966

[4] J.B. Rosser, *Theory and Application of*

$$\int_0^z e^{-x^2}\,dx \text{ and } \int_0^z e^{-p^2y^2}\,dy \int_0^y e^{-x^2}\,dx$$

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[5] V.N. Faddeyeva and N.M. Terent'ev, *Tables of the Values of the Function*

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

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[6] R.E. Greenwood and J.J. Miller, *Zeroes of the Hermite polynomials and weights for Gauss' quatrature formula,* Amer. Math. Soc. Bull., **54**, 765, 1948