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$\int e^{-x^2}dx$ and the Kink Soliton

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Abstract

We provide analytical functions approximating $\int e^{-x^2}dx$, the basis of which is the kink soliton. Because of the accuracy and simplicity of the results (maximum error $< 0.2\%$), it brings new hope that $\int e^{-x^2}dx$ can in fact be written as the sum of simple analytical functions. We demonstrate our results with some applications, particularly to generation of Gaussian random fields without Monte Carlo methods.

1 Introduction

There is an inherent asymmetry between integration and differentiation which makes integration somewhat of an art form, and which is perhaps best exemplified by the apparent lack of an elementary indefinite integral of

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the celebrated Gaussian:

$$\int \exp(\frac{-(x-\beta)^2}{\sigma^2})dx \tag{1}$$

The Gaussian integral is one of the most fundamental, finding applications in statistics, error theory and many branches of physics. In fact, anywhere where one has Gaussian distributions, cummulatives of these distributions will involve the above integral. Only special case definite integrals of e^{-x^2} are known, the most famous being:

$$\int_0^\infty e^{-x^2/\sigma^2} dx = \frac{\sqrt{\pi}\sigma}{2} \tag{2}$$

In addition there is the series expansion [1]:

$$\int_0^x e^{-u^2} du = \sum_{k=1}^{\infty} \frac{(-1)^{k-1} x^{2k-1}}{(k-1)!(2k-1)} \tag{3}$$

Now in practise one can evaluate the integral accurately by numerical quadrature, but in many cases it would be preferable to have an analytical solution. even if it were not exact. as long as the maximum error were very small and the approximation were simple [2]

It turns out that there exists a function well known in analysis of non-linear PDE's whose derivative is very close to Gaussian - the kink soliton:

$$\phi(x) = A\tanh(bx - c\beta) \tag{4}$$

whose derivative is:

$$\chi(x) = Ab\left(1 - \tanh^2(bx - c\beta)\right) \tag{5}$$

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[2]Several rational function approximations exist but they are rather complicated [2].

where A, b, c, and β are all real constants. The graphs of e^{-x^2} and $\chi(x)$ are shown in figure (1). [3] The kink soliton is the positive, time-independent. topological solution to the non-linear $1+1$ dimensional partial differential equation:

$$\phi_{tt} - \phi_{xx} = 2b^2(\phi - \frac{1}{A^2}\phi^3) \tag{6}$$

where a subscript denotes partial derivative with respect to that variable. The solution to this equation is topological because the boundary conditions at $x = \pm\infty$ are different. Leaving the physical origin of ϕ behind, it is interesting to examine the series expansion of $\tanh(x)$:

$$\tanh(x) = \sum_{k=1}^{\infty} \frac{2^{2k}(2^{2k}-1)}{(2k)!} B_{2k} x^{2k-1} \ , \qquad \text{valid for } \ x < \frac{\pi}{2} \tag{7}$$

which should be compared with eq. (3) for $\int e^{-x^2} dx$. Here B_k are the Bernoulli numbers with generating function $t/(e^t - 1)$. We see that although the coefficients differ in each case, the powers of x in the expansions are identical. Further both $\chi(x)$ and e^{-x^2} have the property that their derivatives can be re-expressed in terms of themselves and $\phi(x)$ or powers of x respectively. These observations shed some light on the foundations of the approximation.

[3] One can consider a one-parameter family of approximations to the Gaussian given by replacing $x \to x^\epsilon$ in eq. (5) which give better fits when $\epsilon \neq 1$, but which do not have indefinite integrals as far as is known to the author.

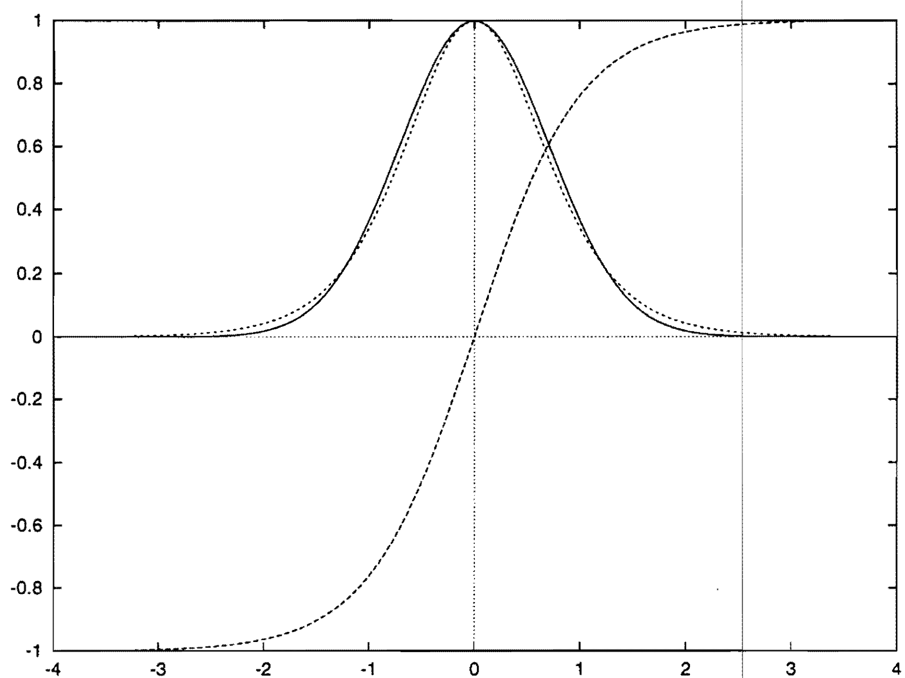

Figure 1: Plot of ϵ^{-x^2} (solid line), $\chi(x)$ (doted line) and $\tanh(x)$ (dashed line) which is the kink soliton.

2 Details of the approximation

Turning to practical issues, we are left with choosing the constants, A, b, c to optimise the approximation of eq. (1). We need three constraints to fix the three parameters. First we require that the Gaussian and $\chi(x)$ have the same symmetry axis. This requires the argument of tanh to vanish at $x_* = \beta$ which immediately implies from eq. (5) that $c = b$.

At this stage we have a choice, dependent on whether we are interested in an approximate solution for small or large x. For large x, a constraint is obviously that our new approximation, $\phi(x)$, must give *exactly* the same result as eq. (2) when differenced at infinity and the origin. This will ensure convergence of our approximation. Since $\tanh(x) \rightarrow 1$ as $x \rightarrow \infty$, and $\tanh(0) = 0$, this implies from eq. (4) that:

$$A = \frac{\sqrt{\pi}\sigma}{2}$$

Finally we can impose that $\chi(x) = e^{-(x-\beta)^2/\sigma^2}$ at some point, i.e. we match the derivatives. We will choose $x = \beta$ as the simplest. This gives:

$$Ab = 1 \Longrightarrow b = \frac{2}{\sqrt{\pi}\sigma}$$

In fact the two are equal at another point as can be seen from figure (1). Our analytical approximation, which is very accurate for large x, is therefore:

$$\phi(x) = \frac{\sqrt{\pi}\sigma}{2} \tanh\left(\frac{2}{\sqrt{\pi}\sigma}(x-\beta)\right) \simeq \int e^{-(x-\beta)^2/\sigma^2} dx \qquad (8)$$

where in this paper $\simeq$ is understood as meaning asymptotic convergence, as $x \rightarrow \infty$ and bounded error $\forall x$. From figures (1,2) we see that the kink derivative underestimates the Gaussian at small $(x-\beta)^2$ and overestimates it at large $(x-\beta)^2$.

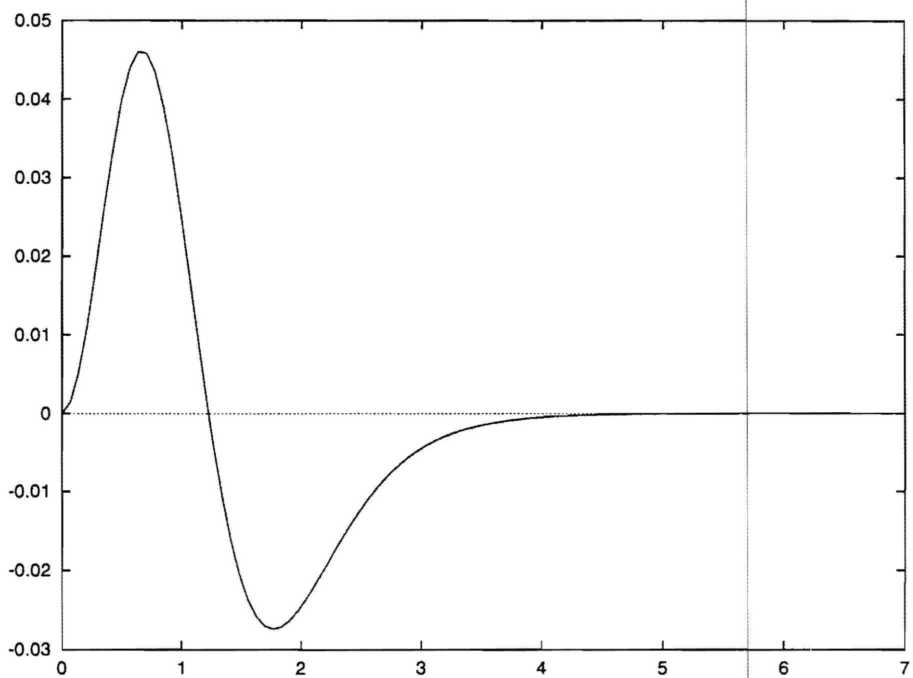

Figure 2: Plot of the difference between e^{-x^2} and $\chi(x)$.

Alternatively if one is interested in $\int_0^u e^{-x^2/\sigma^2} dx$ where $u \leq 4\sigma$ say, then this will not be good enough. since the error in our approximation is strongly confined to small x. Instead we can impose that $\phi(x)$ must give the exact result, not at infinity, but at the end of the interval, i.e. at u. Thus we impose:

$$A \tanh(b(u-\beta)) = \int_0^u e^{-(x-\beta)^2/\sigma^2} dx \tag{9}$$

In addition we need to match the derivatives $\chi(x_*) = e^{-(x_*-\beta)^2/\sigma^2)}$ at some point x_* as before, and then solve the equations for A, b. It is an open ques-

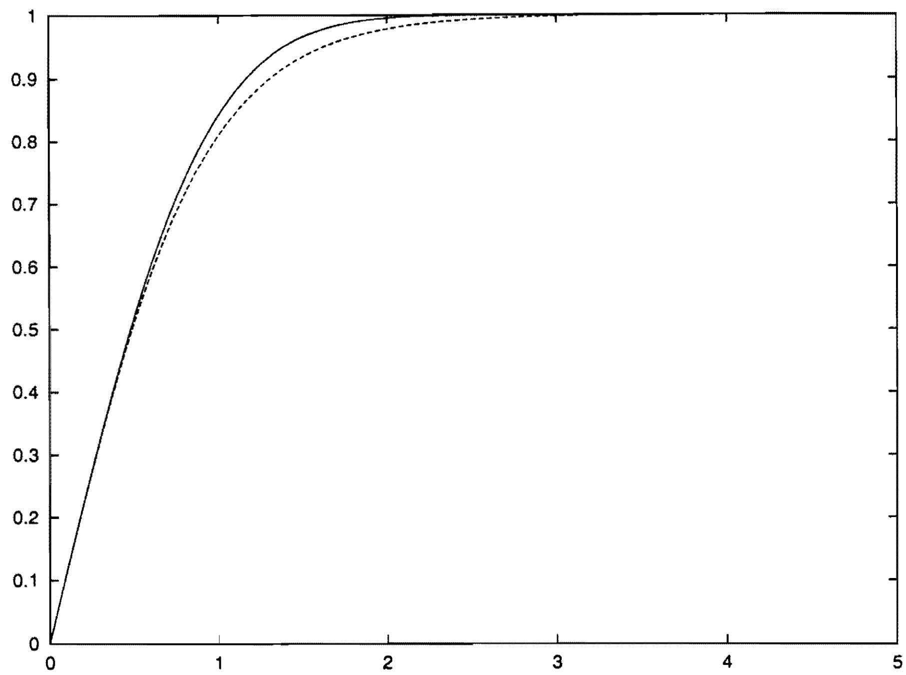

Figure 3: Plot of the error function, soliton approximant, $\phi(x)$. The maximum relative error occurs at $x = 1.12$ and is 3.91%. The error drops below 1% for $x \geq 2.3$ and converges rapidly to zero.

tion which matching point yields the best results. For illustrative purposes we choose $x = \beta$ and again find $A = 1/b$, so that substituting in eq.(9) gives us a nonlinear root-finding problem for A. The right-hand side can be found for example, from tables of the error function, erf(x). This yields an approximation which is exact at $x = u$ and hence a much better approximation for small x, but which is invalid for $x \gg u$. The extension to cases with variable lower limit of integration is obvious and will not be considered.

One might be tempted to generalise eq. (4) to a one-parameter family of approximations to the error function:

$$\Delta_p(x) = A \tanh^p(bx) \tag{10}$$

which have derivative:

$$\Delta_p'(x) = Abp \tanh^{p-1}(bx)\mathrm{sech}^2(bx) \tag{11}$$

However, since for $p \neq 1$, $\Delta_p'(0) = 0$, they are not really suitable as approximations to a Gaussian. Rather they are skewed distributions with maxima at $x > 0$. It turns out however, that they will be useful later.

For testing our approximation we will use the $\phi(x)$ valid for large x, denoted $\phi(x)_L$, given by eq. (8). The crucial question is of course, how good is this approximation ? It turns out that it is very good in most cases, as can be seen from figures (3) and (4). The maximum error from using $\phi(x)_L$ is 3.91% at $x = 1.12$. However as discussed earlier, if one is interested in the result for small x, and x_1 is small, then this is not the best approximation to use. In practise, the error drops off very quickly due to the exponential nature of $\tanh(x)$. For example, the error in estimating $\mathrm{erf}(x)$ drops below 1% for $x \geq 2.3$ and at $x = 5$ the error is 2.51×10^{-5}. The error as a function of x is plotted in figure (4).

3 Does $\int e^{-x^2} dx$ exist in elementary form ?

The shape of figure (4) is, in fact, rather startling because it is a common shape and leads to the conjecture that it can be found *exactly* in terms of elementary functions. From the graph it has a single local maximum and hence two points where the concavity changes. The set of all such functions is very small relative to the set of all smooth functions on **R** but it may not be small enough to ensure that the conjecture is true. Several shapes were tried, such as the log-normal and Poisson distributions, but the best was found to be a generalised Maxwell-distribution:

$$E(x) = \alpha_1 x^n \exp(-\frac{x^2}{\alpha_2}) \tag{12}$$

For the case used in the figures, that of erf(x), the best parameters for reducing the maximum error (i.e. minimising w.r.t. the sup-norm $||\cdot||_\infty$) were (see figure (5)):

$$\alpha_1 = 0.062 \ , \quad n = 2.27 \ , \quad \alpha_2 = 1.43 \tag{13}$$

which reduced the *maximum* error to 0.15%. It would of course be incredible if a function could be found which exactly accounted for the error, proving that $\int e^{-x^2}dx$ existed in elementary form, but even if this is not the case, we have found an accurate and simple solution, erf$(x) = \phi(x) + E(x)$. It is also likely that our choice of function and parameters for $E(x)$ is not optimal, since a formal optimisation was not used, but was based rather on a numerical investigation of the parameter space $\{\alpha_1, \alpha_2, n\}$, which was certainly not exhaustive.

Since the required $E(x)$ is a skewed Gaussian with maximum at non-zero x we can profitably employ the functions given by eq. (11), originally introduced to model the Gaussian, as fits for the error. In this case our approximation becomes:

$$\int_0^x e^{u^2} du = \frac{\sqrt{\pi}}{2}\left[\tanh(\frac{2}{\sqrt{\pi}}x) + (\alpha_3 \tanh^p(x))'\right] \tag{14}$$

where $'$ denotes derivative w.r.t. x. For $\alpha_3 = 0.23$ and $p = 9.7$ the error is at most 9×10^{-3}. By suitable generalisation of the second term it is possible to increase the accuracy to the level of the generalised Maxwell distribution, but for simplicity and because of its suggestiveness, we leave it in the above form.

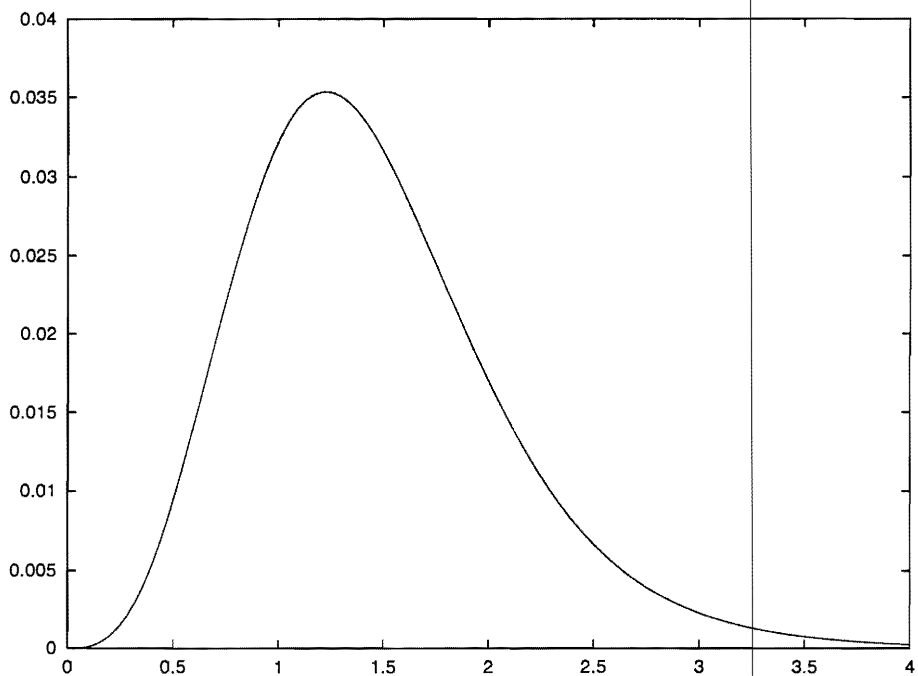

Figure 4: The difference of erf(x) and $\phi(x)_L$. This is closely approximated by log-normal distributions or functions of the form $\alpha_1 x^n e^{-x^2/\alpha_2}$. If this can be fitted exactly by an analytical function then one has the exact integral of e^{-x^2}.

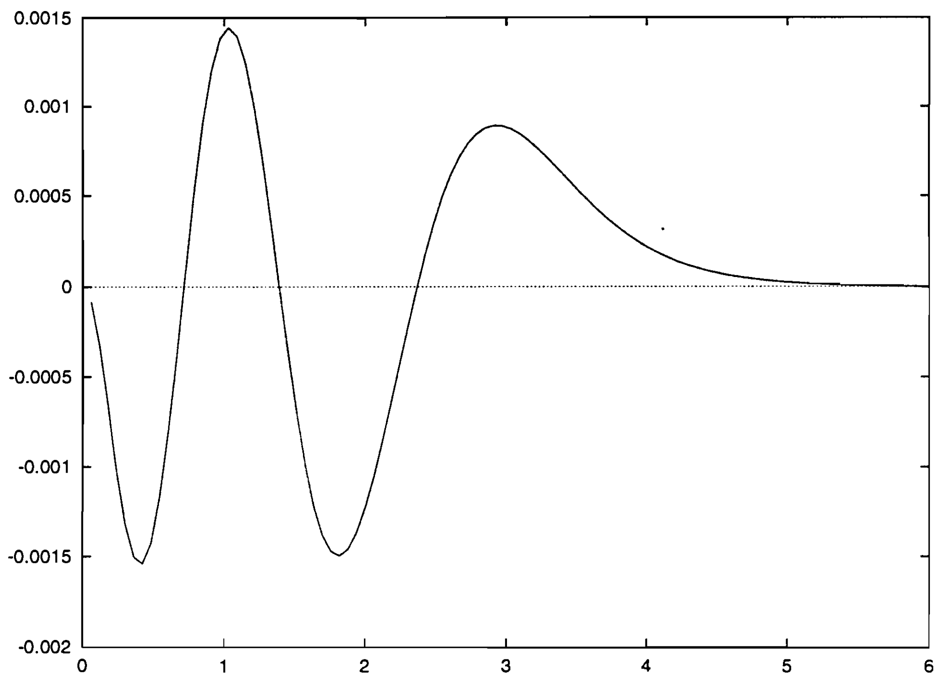

Figure 5: The final error after modeling figure (4) by the generalised Maxwell distribution of eq.(12). The maximum error is about 0.15%.

In the case of the error function we have explicitely that ($\beta = 0$):

$$\mathrm{erf}(x) \simeq \tanh(\frac{2}{\sqrt{\pi}}x) + E(x) \tag{15}$$

where $\mathrm{erf}(x) \equiv \Phi(x) = 2/\sqrt{\pi}\int_0^x e^{-u^2}du$ is the error function. Similarly the complementary error function is given by: $\mathrm{erfc}(x) = 1 - \tanh(\frac{2}{\sqrt{\pi}}x) - E(x)$.

4 Applications

Let us now consider a very small sample of possible applications. A primary example is in the theory of statistics. If we have a uniformly distributed random variable χ and we desire a random variable y with statistics given by a distribution f, first define the integral $F(x) = \int_0^x f(\chi)d\chi$. Then $y = F^{-1}(x)$ will have the same distribution as f, where F^{-1} denotes the inverse of F, on the interval $[F^{-1}(0), F^{-1}(x)]$.

In particular if, as is often the case, we want to generate a realisation of a Gaussian random distribution, $f = \exp(-x^2/\sigma^2)$, then with our approximation, $F(x) = \phi(x)$ (we have dropped the error correction term $E(x)$ for simplicity) and the inverse $\phi^{-1}(x)$, gives us our random variable. In this case if $y = \phi(x)$, then:

$$\phi^{-1}(x) = \frac{\sqrt{\pi}\sigma}{2}\tanh^{-1}(\frac{2}{\sqrt{\pi}\sigma}x) \tag{16}$$

which has the same form as $\phi(x)$ with the replacement $\tanh \rightarrow \tanh^{-1}$ so that both the integral and inverse are essentially trivial. This avoids the necessity of using traditional Monte Carlo methods to calculate Gaussian distributions.

A related problem occurs in the study of structure formation from gravitational collapse from Gaussian initial conditions, a ubiquitous assumption. The Press-Schecter formalism [3], gives the cummulative mass function $f(> M)$, which is the number of objects (such as galaxies) with mass greater than M:

$$f(\geq M) = 1 - \mathrm{erfc}\left(\frac{\delta_c}{\sqrt{2}\sigma(M,z)}\right) \tag{17}$$

where $\delta_c, z \in R$ and σ is the variance of the distribution. This can be found immediately using eq. (15).

Other relations are found from the theory of solutions to the Schrödinger equation with general potential. In particular, for a logarithmic potential we have: (see e.g. [4]) that the wavefunction is determined asymptotically by an integral:

$$\int_0^x \sqrt{h_\ell(u)}du = \sqrt{h_0(x)} + \frac{1}{2}i\sqrt{\pi\lambda}\ \mathrm{erf}(ix^{1/2}) \quad , \qquad x, \lambda \geq 0 \tag{18}$$

where $h_\ell(u) = \ell^2 + \lambda x e^{2x}$. Perhaps the canonical example from quantum theory, however comes from Feynman's path-integral formulation: (we drop $E(x)$ again for simplicity) [1]:

$$\int_u^\infty \exp(-\frac{x^2}{4\delta} - \gamma x)dx \simeq \sqrt{\pi\delta}e^{\delta\gamma^2}\left[1 - \tanh(\frac{2}{\sqrt{\pi}}(\gamma\sqrt{\delta} + \frac{u}{2\sqrt{\delta}}))\right] \tag{19}$$

with $u \to -\infty$.

Further, the error function can be related to special values of the degenerate hypergeometric function, ${}_1F_1(\alpha;\gamma;z)$. In particular:

$$ {}_1F_1(\frac{1}{2};\frac{3}{2};-x^2) \simeq \frac{\sqrt{\pi}}{2x}\tanh(\frac{2}{\sqrt{\pi}}x) $$

Our final example comes from the theory of parabolic cylinder functons, $D_p(z)$, which are solutions to the differential equation:

$$ \frac{d^2u}{dz^2} + (p + \frac{1}{2} - \frac{z^2}{4})u = 0 \tag{20} $$

with $u = D_p(z)$ and for integer values of $p = n$, they are related to the Hermite polynomials, $H_n(z)$ by $D_n(z) = 2^{-n/2}e^{-z^2/4}H_n(\frac{z}{\sqrt{2}})$. Finally we may write, for the special cases of $n = -1, -2$:

$$ D_{-1}(z) \simeq e^{z^2/4}\sqrt{\frac{\pi}{2}}\left[1 - \tanh(\sqrt{\frac{2}{\pi}}z)\right] \tag{21} $$

$$ D_{-2}(z) \simeq -e^{z^2/4}\sqrt{\frac{\pi}{2}}\left[\sqrt{\frac{2}{\pi}}e^{-z^2/2} - z(1 - \tanh(\sqrt{\frac{2}{\pi}}z))\right] \tag{22} $$

$$ \tag{23} $$

These represent an extremely small range of perhaps fairly trivial applications, apart from the discussion of generating Gaussian random fields, and it is hoped that there are more useful applications unknown to the author, where it is truly useful to have an approximate analytical expression for $\int e^{-x^2}dx$.

5 Conclusions

In this *Letter* we have presented a function approximating erf(x) to better than 4% $\forall\ x$, with exponential convergence as $x \to \infty$. This solution is simply the kink soliton. $\phi(x) = \tanh(2x/\sqrt{\pi})$.

Further we have found a solution with maximum error of 0.15% by adding a generalised Maxwell distribution to the kink soliton, equations (12), (14). This leads us to conjecture that $\int e^{-x^2} dx$ exists in elementary form. Future work should be aimed at finding truly optimal solutions. Finally applications were suggested, particularly to the simple generation of Gaussian random fields without Monte Carlo methods.

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