# A note on simple approximations of Gaussian type integrals with applications

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**Abstract**

In this note, we introduce new simple approximations for Gaussian type integrals. A key ingredient is the approximation of the function $e^{-x^2}$ by sum of three simple polynomial-exponential functions. Five special Gaussian type integrals are then considered as applications. Approximation of the Voigt error function is investigated.

*Keywords:* Exponential approximation, Gauss integral type function, Voigt error function.

## 1. Motivation

Gaussian type integrals play a central role in various branches of mathematics (probability theory, statistics, theory of errors . . . ) and physics (heat and mass transfer, atmospheric science. . . ). The most famous example of this class of integrals is the Gauss error function defined by $\operatorname{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} dx$. As for the $\operatorname{erf}(y)$, plethora of useful Gaussian type integral have no analytical expression. For this reason, a lot of an approximations have been developed, more or less complicated, with more or less precision (for the $\operatorname{erf}(y)$ function, see [4] and the references therein).

In this paper, we aim to provide acceptable and simple approximations for possible sophisticated Gaussian type integrals. We follow the simple approach of [1] which consists in expressing the function $e^{-x^2}$ as a finite sum of $N$ functions having a more tractable polynomial-exponential form: $\alpha_n |x|^n e^{-\beta_n |x|}$, where $\alpha_n$ and $\beta_n$ are real numbers and $n \in \{0, \ldots, N\}$, i.e. $e^{-x^2} \approx \sum_{n=0}^{N} \alpha_n |x|^n e^{-\beta_n |x|}$. The challenge is to chose $\alpha_0, \ldots, \alpha_N$ and $\beta_0, \ldots, \beta_N$ such that the rest function $\epsilon(x) = e^{-x^2} - \sum_{n=0}^{N} \alpha_n |x|^n e^{-\beta_n |x|}$ is supposed to be small: $|\epsilon(x)| << 1$. With such a choices, for a function $g(x,t)$, the following approximation is acceptable:

$$\int_{-\infty}^{+\infty} g(x,t) e^{-x^2} dx \approx \sum_{n=0}^{N} \alpha_n \int_{-\infty}^{+\infty} |x|^n e^{-\beta_n |x|} g(x,t) dx,$$

assuming that the integrals exist and with the idea in mind that the integral terms in the sum have analytical expressions. Considering $N = 1$, it is shown in [1] that, for $\gamma = 2.75$, we have $e^{-x^2} \approx e^{-2\gamma|x|} + 2\gamma|x|e^{-\gamma|x|}$, so $\alpha_0 = 1$, $\alpha_1 = 2\gamma$, $\beta_0 = 2\gamma$, $\beta_1 = \gamma$. With this set of coefficients, [1] shown that the rest function $\epsilon_1(x) = e^{-x^2} - \left(e^{-2\gamma|x|} + 2\gamma|x|e^{-\gamma|x|}\right)$ has a reasonably small magnitude: $|\epsilon_1(x)| < 0.032$ (value obtained using the Faddeeva Package [2] which includes a wrapper for MATLAB). Using this result, [1] shows a simple rational approximation a Gaussian type integral, named the Voigt error function. Contrary to more accurate approximations, it has the advantage to be simple and very useful for rapid computation when dealing with large-scale data. In this study, we propose to explore this approach by considering an additional polynomial-exponential function, with polynomial of degree 2; the case $N = 2$ is considered. We determine suitable coefficients $\alpha_0, \alpha_1, \alpha_2$ and $\beta_0, \beta_1, \beta_2$ to obtain a rest function with a smaller magnitude to the one of $\epsilon_1(x)$ evaluated by [1]. We then use this approximation to show simple approximations for complex Gaussian type integrals, including the

Voigt error function. This paper is organized as follows. In Section 2, we present our approximation results. Applications are given for the Voigt error function in Section 3.

## 2. Gaussian integral type approximations

Let us recall that we consider the approximation :

$$e^{-x^2} \approx \sum_{n=0}^{N} \alpha_n |x|^n e^{-\beta_n |x|},$$

with a focus on the case $N = 2$. After an empiric study, a correct fit is given with the following coefficients:

$$\alpha_0 = 1, \quad \alpha_1 = 4\theta, \quad \alpha_2 = 4\theta^2, \quad \beta_0 = 4\theta, \quad \beta_1 = 3\theta, \quad \beta_2 = 2\theta,$$

with $\theta = 1.885$. For a given mathematical context, an optimal choice can be done using specific criteria, for example using a simple grid search. For this special configuration, observe that we have

$$e^{-x^2} \approx e^{-4\theta|x|} + 4\theta|x|e^{-3\theta|x|} + 4\theta^2 x^2 e^{-2\theta|x|} = \left(e^{-2\theta|x|} + 2\theta|x|e^{-\theta|x|}\right)^2. \tag{1}$$

With this setting, the rest function $\epsilon_2(x) = e^{-x^2} - \left(4\theta^2 x^2 e^{-2\theta|x|} + 4\theta|x|e^{-3\theta|x|} + e^{-4\theta|x|}\right)$ has a reasonably small magnitude; we have $|\epsilon_2(x)| < 0.018$ (using the same reference code). Note that the upper bound 0.018 is (near twice) smaller to the upper bound of $|\epsilon_1(x)|$ studied in [1]. Superposition of the rest functions $\epsilon_1(x)$ and $\epsilon_2(x)$ is given in Figure 1. We see that for a small interval around 0, the error

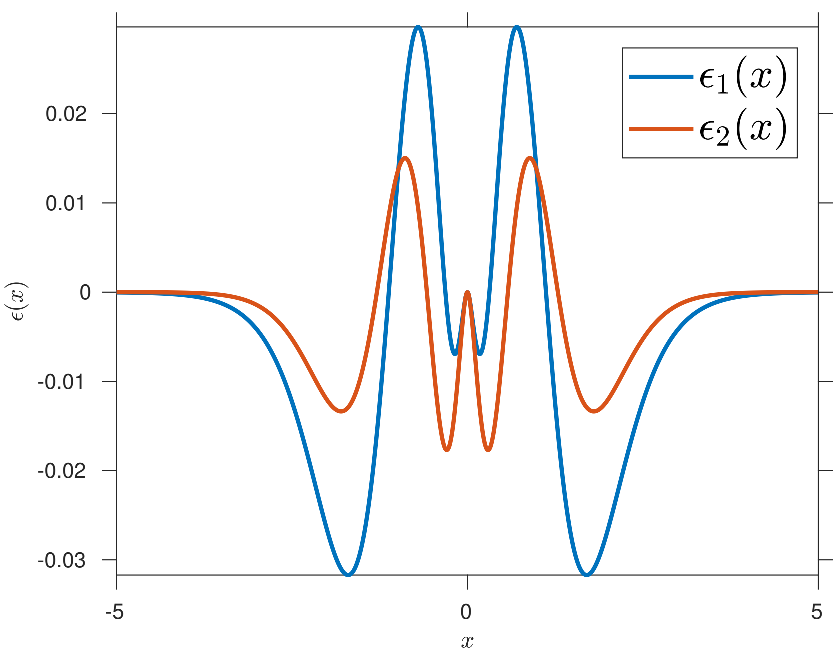


Figure 1: Graphical comparison of $\epsilon_1(x)$ and $\epsilon_2(x)$

$\epsilon_1(x)$ is smaller to $\epsilon_2(x)$, but $\epsilon_2(x)$ is globally the smallest. Indeed, we have $\int_{-5}^{5} |\epsilon_2(x)|dx \approx 0.05240866$ with an absolute error less than 0.00012 against $\int_{-5}^{5} |\epsilon_1(x)|dx \approx 0.1050965$ with an absolute error less than 0.00011. Therefore, for a wide class of functions $g(x,t)$, we have :

$$\int_{-\infty}^{+\infty} g(x,t)e^{-x^2}dx \approx \sum_{n=0}^{N} \alpha_n \int_{-\infty}^{+\infty} |x|^n e^{-\beta_n|x|} g(x,t)dx,$$

We then use this result to approximate several nontrivial Gaussian type integrals (define on the semi-finite interval $(0, +\infty)$). Let $\nu > -1$, $\mu \geq 0$ and $p \geq 0$. We consider the following coefficients:

$$\alpha_{0,p} = 1, \quad \alpha_{1,p} = 4\theta\sqrt{p}, \quad \alpha_{2,p} = 4\theta^2 p, \quad \beta_{0,p} = 4\theta\sqrt{p}, \quad \beta_{1,p} = 3\theta\sqrt{p}, \quad \beta_{2,p} = 2\theta\sqrt{p},$$

in such a way that our previous approximation gives: $e^{-px^2} \approx \sum_{n=0}^{N} \alpha_{n,p}|x|^n e^{-\beta_{n,p}|x|}$. Then we have the following approximations, provided chosen $\nu$, $\mu$ and $p$ such that they exist:

**Integral approximation I.** Using our approximation and [3, Case 3, Subsection 5.3], we have

$$\int_0^{+\infty} x^\nu e^{-\mu x} e^{-px^2} dx \approx \sum_{n=0}^{2} \alpha_{n,p} \frac{\Gamma(n+\nu+1)}{(\beta_{n,p}+\mu)^{n+\nu+1}}.$$

**Integral approximation II.** Using our approximation and [3, Case 7, Subsection 5.5], we have

$$\int_0^{+\infty} x^\nu \ln(x) e^{-px^2} dx \approx \sum_{n=0}^{2} \alpha_{n,p} \frac{\Gamma(n+\nu+1)}{(\beta_{n,p})^{n+\nu+1}} \left[\psi(n+\nu+1) - \ln(\beta_{n,p})\right],$$

where $\psi(x)$ is the digamma function, i.e. the logarithmic derivative of the gamma function.

**Integral approximation III.** Using our approximation and [3, Case 12, Subsection 5.3], we have

$$\int_0^{+\infty} x^\nu e^{-\frac{\mu}{x}} e^{-px^2} dx \approx \sum_{n=0}^{2} \alpha_{n,p} 2 \left(\frac{\mu}{\beta_{n,p}}\right)^{(\nu+n+1)/2} K_{n+\nu+1}(2\sqrt{\mu\beta_{n,p}}),$$

where $K_a(x)$ is the modified Bessel function of the second kind with parameter $a$.

**Integral approximation IV.** Using our approximation and [3, Case 7, Subsection 7.3], we have

$$\int_0^{+\infty} x^\nu \cos(\upsilon x) e^{-\mu x} e^{-px^2} dx \approx$$
$$\sum_{n=0}^{2} \alpha_{n,p}\Gamma(n+\nu+1) \left[(\beta_{n,p}+\mu)^2 + \upsilon^2\right]^{-(n+\nu+1)/2} \cos\left[(\nu+n+1)\arctan\left(\frac{\upsilon}{\beta_{n,p}+\mu}\right)\right]. \tag{2}$$

Let us remark that if we take $\upsilon = 0$, we rediscover Integral approximation I.

**Integral approximation V.** Using our approximation and [3, Case 8, Subsection 8.3], we have

$$\int_0^{+\infty} x^\nu \sin(\upsilon x) e^{-\mu x} e^{-px^2} dx \approx$$
$$\sum_{n=0}^{2} \alpha_{n,p}\Gamma(n+\nu+1) \left[(\beta_{n,p}+\mu)^2 + \upsilon^2\right]^{-(n+\nu+1)/2} \sin\left[(\nu+n+1)\arctan\left(\frac{\upsilon}{\beta_{n,p}+\mu}\right)\right]. \tag{3}$$

These approximations can be useful in many domains of applied mathematics. In the next section, we illustrate the approximations (2) and (3) by investigate approximation of the Voigt error function, also considered in [1] for comparison. Note that given the approximation of $e^{-x^2}$, one can also compute Fresnel integrals, and similar related functions as well, such as other complex error functions.

## 3. Application to the Voigt error function

The Voigt error function can be defined as $w(x,y) = K(x,y) + iL(x,y)$ where

$$K(x,y) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-\frac{t^2}{4}} e^{-yt} \cos(xt)dt, \qquad L(x,y) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-\frac{t^2}{4}} e^{-yt} \sin(xt)dt.$$

Clearly, $K(x,y)$ and $L(x,y)$ belongs to the family of Gaussian type integrals. Further details on the Voigt error function and its numerous applications are given in [5] and [1]. It follows from the approximation (2) with the notations : $p = \frac{1}{4}$, $\mu = y$ and $\upsilon = x$, that

$$\begin{aligned} K(x,y) &\approx \frac{1}{\sqrt{\pi}} \Bigg[ \left[(y+2\theta)^2 + x^2\right]^{-\frac{1}{2}} \cos\left[\arctan\left(\frac{x}{y+2\theta}\right)\right] \\ &+ 2\theta \left(\left(y + \frac{3}{2}\theta\right)^2 + x^2\right)^{-1} \cos\left[2\arctan\left(\frac{x}{y+\frac{3}{2}\theta}\right)\right] \\ &+ 2\theta^2 \left((y+\theta)^2 + x^2\right)^{-\frac{3}{2}} \cos\left[3\arctan\left(\frac{x}{y+\theta}\right)\right]\Bigg] \end{aligned}$$

and, by the approximation (3), we have the same expression for $L(x,y)$ but with sin instead of cos :

$$\begin{aligned} L(x,y) &\approx \frac{1}{\sqrt{\pi}} \Bigg[ \left[(y+2\theta)^2 + x^2\right]^{-\frac{1}{2}} \sin\left[\arctan\left(\frac{x}{y+2\theta}\right)\right] \\ &+ 2\theta \left(\left(y + \frac{3}{2}\theta\right)^2 + x^2\right)^{-1} \sin\left[2\arctan\left(\frac{x}{y+\frac{3}{2}\theta}\right)\right] \\ &+ 2\theta^2 \left((y+\theta)^2 + x^2\right)^{-\frac{3}{2}} \sin\left[3\arctan\left(\frac{x}{y+\theta}\right)\right]\Bigg]. \end{aligned}$$

Let us recall some trigonometric formulas: we have $\cos(\arctan(x)) = \frac{1}{\sqrt{1+x^2}}$, $\cos(2\arctan(x)) = \frac{1-x^2}{1+x^2}$, $\cos(3\arctan(x)) = \frac{1-3x^2}{(1+x^2)^{\frac{3}{2}}}$, $\sin(\arctan(x)) = \frac{x}{\sqrt{1+x^2}}$, $\sin(2\arctan(x)) = \frac{2x}{1+x^2}$, $\sin(3\arctan(x)) = \frac{x(3-x^2)}{(1+x^2)^{\frac{3}{2}}}$. Using these formulas in the previous approximations of $K(x,y)$ and $L(x,y)$, we obtain :

$$K(x,y) \approx \frac{1}{\sqrt{\pi}} \left[ \frac{y+2\theta}{(y+2\theta)^2 + x^2} + 2\theta \frac{(y+\frac{3}{2}\theta)^2 - x^2}{\left(\left(y+\frac{3}{2}\theta\right)^2 + x^2\right)^2} + 2\theta^2 (y+\theta) \frac{(y+\theta)^2 - 3x^2}{\left((y+\theta)^2 + x^2\right)^3} \right]$$

and

$$L(x,y) \approx \frac{1}{\sqrt{\pi}} \left[ \frac{x}{(y+2\theta)^2 + x^2} + 4\theta \left(y + \frac{3}{2}\theta\right) \frac{x}{\left(\left(y+\frac{3}{2}\theta\right)^2 + x^2\right)^2} + 2\theta^2 \frac{x(3(y+\theta)^2 - x^2)}{\left((y+\theta)^2 + x^2\right)^3} \right].$$

Let us denote by $K_{\mathrm{app}_2}(x,y)$ and $L_{\mathrm{app}_2}(x,y)$ the approximation above for $K(x,y)$ and $L(x,y)$ respectively. On the other side, we denote by $K_{\mathrm{app}_1}(x,y)$ and $L_{\mathrm{app}_1}(x,y)$ the approximation for $K(x,y)$ and $L(x,y)$ respectively proposed by [1]. The errors of the obtained approximations can be evaluated using the absolute differences for the real and imaginary parts of the complex error function defined by

$$\Delta_{\mathrm{Re}_*} = |K_{\mathrm{app}_*}(x,y) - K(x,y)|, \qquad \Delta_{\mathrm{Im}_*} = |L_{\mathrm{app}_*}(x,y) - L(x,y)|.$$

As references for $K(x,y)$ and $L(x,y)$ functions we used [2] which provide highly accurate results. In order to have a visual overview of the behaviour of these error functions, the curves of $\Delta_{\mathrm{Re}_*}$ and $\Delta_{\mathrm{Im}_*}$ are given in Figure 2. For both approximation error functions, the maximal discrepancy is observed at $y = 0$, more precisely, we have: $\max(\Delta_{\mathrm{Re}_1}) \approx 0.0337, \max(\Delta_{\mathrm{Im}_1}) \approx 0.0349$ and $\max(\Delta_{\mathrm{Re}_2}) \approx 0.0168, \max(\Delta_{\mathrm{Im}_2}) \approx 0.0138$. Therefore, the approximation we propose is about twice as accurate as the one proposed in [1] while maintaining its simplicity and computational advantages.

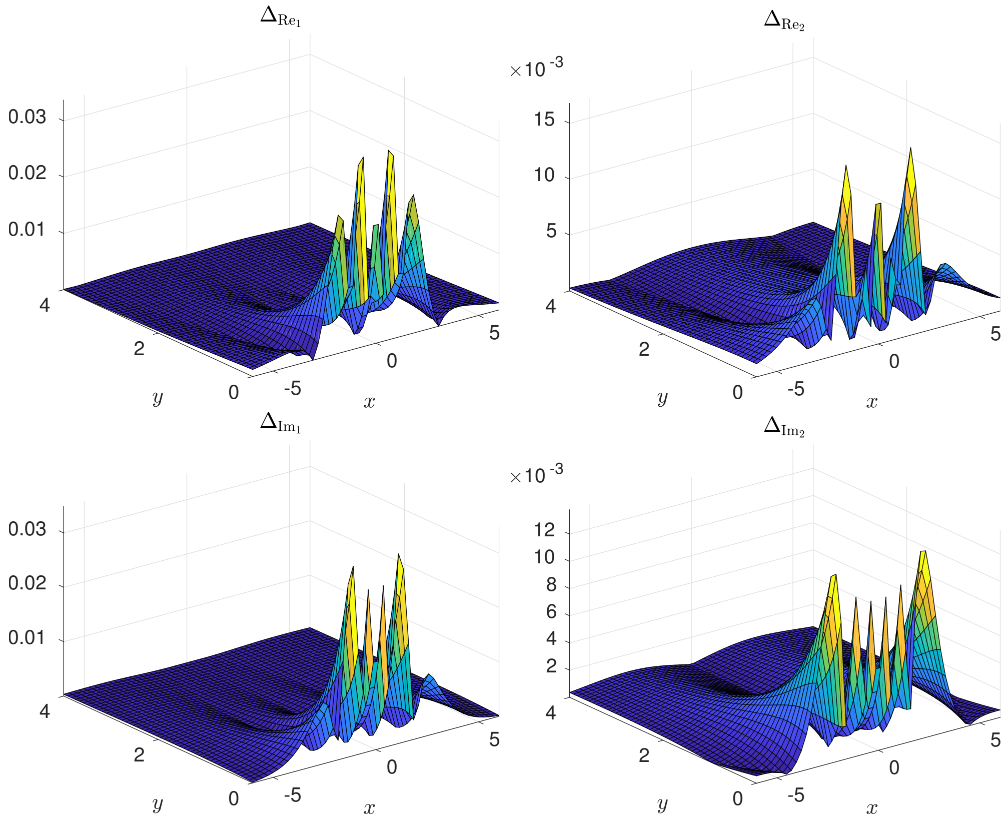


Figure 2: Graphical comparison of $\Delta_{\mathrm{Re}_*}$ and $\Delta_{\mathrm{Im}_*}$.


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