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On some applicable approximations of Gaussian type integrals

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

Keywords: Exponential approximation, Gauss integral type function, Voigt error function.
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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 approximations have been

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developed, more or less complicated, with more or less precision (for the $\mathrm{erf}(y)$ function, see [6] and the references therein).

In this paper, we aim to provide acceptable and applicable 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 α_n and β_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 choose $\alpha_0, \ldots, \alpha_N$ 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: $|\epsilon(x)| \ll 1$. With such a choice, 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 [3] 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 polynomials 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 applicable 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. Concluding remarks are given in Section 4.

2 Gaussian integral type approximations

2.1 Approximation result

Our main result is the following approximation.

Claim. *The following approximation for e^{-x^2} is sharp:*

$$e^{-x^2} \approx \sum_{n=0}^{2} \alpha_n |x|^n e^{-\beta_n |x|}, \tag{1}$$

with $\alpha_0 = 1$, $\alpha_1 = 4\theta$, $\alpha_2 = 4\theta^2$, $\beta_0 = 4\theta$, $\beta_1 = 3\theta$, $\beta_2 = 2\theta$ *and* $\theta = 1.885$.

One can notice that the definitions of α_0, α_1, α_2, β_0, β_1 and β_2 are such that

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

The sharpness of our approximation can be shown in various ways. In particular, one can show that the rest function given by

$$\epsilon_2(x) = e^{-x^2} - \left(4\theta^2 x^2 e^{-2\theta|x|} + 4\theta|x|e^{-3\theta|x|} + e^{-4\theta|x|}\right)$$

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 $\epsilon_1(x)$ 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.

Also, let us mention that exponential of a homogeneous polynomial can be approximate in a similar way by using composition. For instance, for e^{-x^4}, we can write

$$e^{-x^4} \approx \sum_{n=0}^{2} \alpha_n x^{2n} e^{-\beta_n x^2}, \approx \sum_{n=0}^{2}\sum_{m=0}^{2} \alpha_n \alpha_m \beta_n^{m/2} |x|^{m+2n} e^{-\beta_m \sqrt{\beta_n}|x|}.$$

2.2 Approximation of Gaussian type integrals

It follows from (1) that, for a wide class of functions $g(x,t)$, we have the following integral approximation:

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

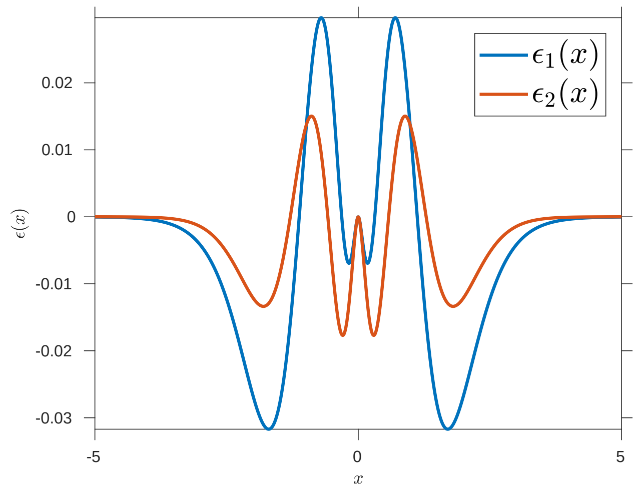

Figure 1: Graphical comparison of $\epsilon_1(x)$ and $\epsilon_2(x)$.

We propose to use this result to approximate several nontrivial Gaussian type integrals (define on the semi-finite interval $(0, +\infty)$). Most of them do not have a close form and do not belong to the list of Gaussian-type integrals by [4].

Let $\nu > -1$, $\mu \geq 0$ and $p \geq 0$. Then, it follows from (1) that

$$e^{-px^2} \approx \sum_{n=0}^{2} \alpha_{n,p} |x|^n e^{-\beta_{n,p}|x|},$$

with $\alpha_{0,p} = 1$, $\alpha_{1,p} = 4\theta\sqrt{p}$, $\alpha_{2,p} = 4\theta^2 p$, $\beta_{0,p} = 4\theta\sqrt{p}$, $\beta_{1,p} = 3\theta\sqrt{p}$, $\beta_{2,p} = 2\theta\sqrt{p}$ and $\theta = 1.885$. Then, we have the following approximations, provided chosen ν, μ and p such that the integrals exist:

Integral approximation I. Using our approximation and [5, 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 [5, 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 [5, 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 [5, Case 7, Subsection 7.3], we have

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

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

Integral approximation V. Using our approximation and [5, Case 8, Subsection 8.3], we have

$$\begin{aligned}\int_0^{+\infty} & x^\nu \sin(\upsilon x) e^{-\mu x} e^{-px^2} dx \approx \\ & \sum_{n=0}^{2} \alpha_{n,p} \Gamma(n+\nu+1) \left[(\beta_{n,p}+\mu)^2 + \upsilon^2\right]^{-(n+\nu+1)/2} \times \\ & \sin\left[(\nu+n+1)\arctan\left(\frac{\upsilon}{\beta_{n,p}+\mu}\right)\right]. \end{aligned} \tag{4}$$

These approximations can be useful in many domains of applied mathematics. In the next section, we illustrate the approximations (3) and (4) 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 $w(x,y) = K(x,y) + iL(x,y)$, $x \in \mathbb{R}$ and $y > 0$, where

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

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 [2], [7] and [1]. It follows from the approximation (3) with the notations: $p = 1/4$, $\mu = y$ 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 (4), 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

$$\begin{aligned} \cos(\arctan(x)) &= 1/\sqrt{1+x^2}, \quad \cos(2\arctan(x)) = (1-x^2)/(1+x^2), \\ \cos(3\arctan(x)) &= (1-3x^2)/(1+x^2)^{3/2}, \quad \sin(\arctan(x)) = x/\sqrt{1+x^2}, \\ \sin(2\arctan(x)) &= 2x/1+x^2, \quad \sin(3\arctan(x)) = x(3-x^2)/(1+x^2)^{3/2}. \end{aligned}$$

Using these formulas in the previous approximations of $K(x,y)$ and $L(x,y)$, we obtain:

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

and

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

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 [3] which provide highly accurate results. In order to have a visual overview of the behavior of these error functions, the curves of Δ_{Re_*} and Δ_{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.

4 Conclusion

In this paper, we provide a contribution to the applicable approximations area. We propose a sharp approximation of the important function e^{-x^2} with simple polynomial-exponential functions and use it to present tractable approximations of complex Gaussian integrals. An application to the Voigt error function is provided to illustrate the usefulness of our approximation.

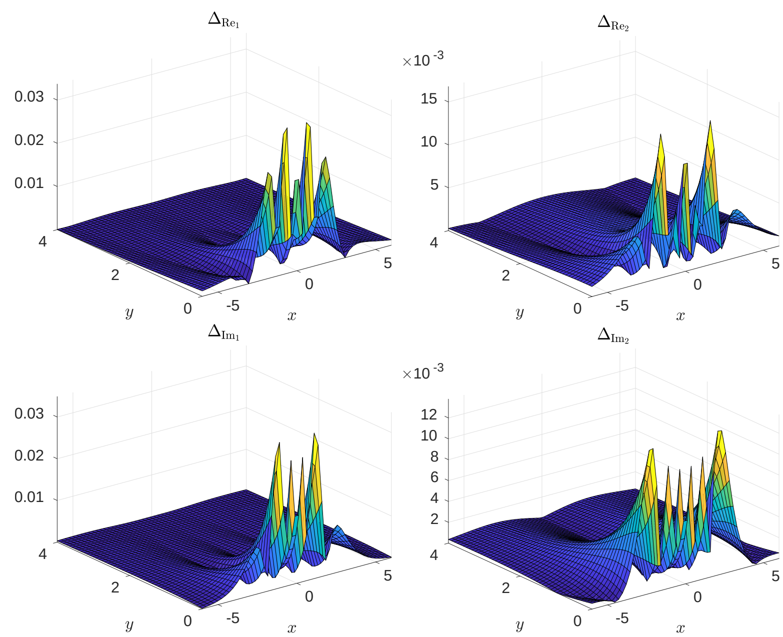

Figure 2: Graphical comparison of Δ_{Re_*} and Δ_{Im_*}.

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