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LETTER TO THE EDITOR

A new series for approximating Voigt functions*

John A Gubner†

Department of Electrical and Computer Engineering, University of Wisconsin, Madison, WI 53706, USA

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Abstract. A Voigt function is the convolution of a Gaussian and a Cauchy, or Lorentzian, density. The computation of these functions is required in problems arising in a variety of subjects such as nuclear reactors, atmospheric transmittance, and spectroscopy. This letter presents a new series for the approximate computation of Voigt functions. The derivation is accomplished using straightforward Fourier techniques, and it yields computable error bounds between the approximation and the Voigt function. The approach also permits a simple derivation of an asymptotic expansion for large argument values.

The convolution of a Gaussian probability density and a Cauchy, or Lorentzian, probability density is known as a Voigt function. Because Voigt functions arise in many different contexts, such as nuclear reactor theory, atmospheric transmittance, and spectroscopy, there has been much interest in computing them, e.g. [1, 4–11].

In the present letter we derive a simple new series approximation for Voigt functions along with computable error bounds in section 2. We also give a simple derivation of an asymptotic expansion with error bounds in section 3 and a numerical example is discussed in section 4.

The standard Gaussian and Lorentzian probability densities are $G(\theta) := \mathrm{e}^{-\theta^2/2}/\sqrt{2\pi}$ and $L(\theta) := 1/[\pi(1+\theta^2)]$, respectively. The Voigt function can be written as

$$h(z,\alpha) := \int_{-\infty}^{\infty} G(z-\alpha\theta)L(\theta)\,\mathrm{d}\theta\,. \tag{1}$$

Since $h(z,0) = G(z)$, our interest is in the case $\alpha > 0$.

A new series for h

We derive the approximation of $h(z,\alpha)$,

$$\tilde{h}_{W,N}(z,\alpha) := \sqrt{\frac{2}{\pi}}\frac{1}{W}\sum_{n=-N}^{N} \mathrm{e}^{-2(\pi/W)^2n^2} I_n(z,\alpha,W) \tag{2}$$

where

$$I_n(z,\alpha,W) := \mathrm{Re}\left[\frac{1-(-1)^n\mathrm{e}^{(-W/2)(\alpha+\mathrm{i}z)}}{\alpha+\mathrm{i}(z-n2\pi/W)}\right]. \tag{3}$$

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† E-mail address: gubner@engr.wisc.edu

Given any $\alpha_{\min} > 0$, we show that the approximation error, $|h(z,\alpha) - \tilde{h}_{W,N}(z,\alpha)|$, is uniformly bounded for all z and all $\alpha \geqslant \alpha_{\min}$. We also give computable bounds on the error as a function of W and N.

To establish our claims, we proceed as follows. We begin by taking Fourier transforms of (1), regarded as functions of z. This results in

$$\hat{h}(\omega,\alpha) := \int_{-\infty}^{\infty} h(z,\alpha)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z = \widehat{G}(\omega)\widehat{L}(\alpha\omega)$$

where $\widehat{G}(\omega) = \mathrm{e}^{-\omega^2/2}$ and $\widehat{L}(\alpha\omega) = \mathrm{e}^{-\alpha|\omega|}$. It then follows that

$$h(z,\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{G}(\omega)\widehat{L}(\alpha\omega)\mathrm{e}^{-\mathrm{i}\omega z}\,\mathrm{d}\omega\,. \tag{4}$$

In particular, $h(0,\alpha) = \pi^{-1}\mathrm{e}^{\alpha^2/2}\int_\alpha^\infty \mathrm{e}^{-\omega^2/2}\,\mathrm{d}\omega$, which can be evaluated in terms of the complementary error function. For $W > 0$ put

$$h_W(z,\alpha) := \frac{1}{2\pi}\int_{-W/2}^{W/2} \widehat{G}(\omega)\widehat{L}(\alpha\omega)\mathrm{e}^{-\mathrm{i}\omega z}\,\mathrm{d}\omega\,. \tag{5}$$

For $\alpha \geqslant \alpha_{\min}$,

$$|h(z,\alpha) - h_W(z,\alpha)| \leqslant \frac{\mathrm{e}^{\alpha_{\min}^2/2}}{\pi}\int_{W/2+\alpha_{\min}}^{\infty} \mathrm{e}^{-\omega^2/2}\,\mathrm{d}\omega \tag{6}$$

which is a decreasing function of $\alpha_{\min}$. Also, the bound is exact for $z = 0$ and $\alpha = \alpha_{\min}$.

Since the integral in (5) is over a finite interval, and since $\widehat{G}$ is continuously differentiable with $\widehat{G}(W/2) = \widehat{G}(-W/2)$, $\widehat{G}$ has a uniformly convergent Fourier series [3, p 321–2]. We can therefore replace $\widehat{G}(\omega)$ in (5) by its Fourier series, $\sum_{n=-\infty}^{\infty}\hat{g}_n\mathrm{e}^{\mathrm{i}nz_0\omega}$, where $z_0 := 2\pi/W$, and

$$\hat{g}_n = \frac{1}{W}\int_{-W/2}^{W/2} \widehat{G}(\omega)\mathrm{e}^{-\mathrm{i}nz_0\omega}\,\mathrm{d}\omega\,. \tag{7}$$

Since

$$\tfrac{1}{2}\int_{-W/2}^{W/2} \widehat{L}(\alpha\omega)\mathrm{e}^{-\mathrm{i}\omega(z-nz_0)}\,\mathrm{d}\omega \tag{8}$$

is equal to $I_n(z,\alpha,W)$ in (3), we find that

$$h_W(z,\alpha) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty}\hat{g}_n\, I_n(z,\alpha,W)\,.$$

Now put

$$h_{W,N}(z,\alpha) := \frac{1}{\pi}\sum_{n=-N}^{N}\hat{g}_n\, I_n(z,\alpha,W)\,. \tag{9}$$

We show in the appendix that

$$|h_W(z,\alpha) - h_{W,N}(z,\alpha)| \leqslant \frac{C_N(W)}{Nz_0^2\alpha_{\min}} \tag{10}$$

where

$$C_N(W) := \frac{2}{\pi}\left[\mathrm{e}^{-W^2/8} + 2\overline{K}_N(W)/W\right]$$

and

$$\overline{K}_N(W) := \sup_{n>N}\left|\int_0^{W/2} \widehat{G}''(\omega)\cos(nz_0\omega)\,\mathrm{d}\omega\right|. \tag{11}$$

Note that by the Riemann–Lebesgue lemma [2, p 80], $\overline{K}_N(W) \to 0$ as $N \to \infty$.

We have now proved that for any z and any $\alpha > 0$, $\lim_{W\to\infty}\left[\lim_{N\to\infty} h_{W,N}(z,\alpha)\right] = h(z,\alpha)$. In practice, W and N are finite, and we now show that $h_{W,N}$ can be approximated by $\tilde{h}_{W,N}$ as follows. If W is large, then (7) tells us that $\hat{g}_n \approx (2\pi/W)G(nz_0)$. Making this substitution in (9) yields the right-hand side of (2). To bound the error in making this substitution, observe that

$$|\hat{g}_n - (2\pi/W)G(nz_0)| \leqslant \frac{2}{W}\int_{W/2}^{\infty} \mathrm{e}^{-\omega^2/2}\,\mathrm{d}\omega. \tag{12}$$

Now, by (8), $|I_n(z,\alpha,W)| \leqslant 1/\alpha$, and thus

$$|h_{W,N}(z,\alpha) - \tilde{h}_{W,N}(z,\alpha)| \;\leqslant\; \frac{2N+1}{\pi\alpha_{\min}}\frac{2}{W}\int_{W/2}^{\infty} \mathrm{e}^{-\omega^2/2}\,\mathrm{d}\omega. \tag{13}$$

By combining (6), (10) and (13), we have a uniform bound on the absolute error, $|h(z,\alpha) - \tilde{h}_{W,N}(z,\alpha)|$, for all z and all $\alpha \geqslant \alpha_{\min}$.

Remark. From (6), (10), and (13), we see that our approximation guarantees more accuracy as $\alpha_{\min}$ increases.

Asymptotic expansion of h

We have shown that for fixed W and N, $\tilde{h}_{W,N}(z,\alpha)$ can uniformly approximate $h(z,\alpha)$. However, from (4) and the Riemann–Lebesgue lemma, we see that for fixed α, as $|z| \to \infty$, $h(z,\alpha) \to 0$. This decay is also exhibited by the approximation in (2) and (3). Hence, for large $|z|$, the bounds on the approximation error may be greater than the magnitude of the number we are trying to compute. Therefore, in this section we present an asymptotic expansion $\overline{h}_n(z,\alpha)$ that becomes more accurate as $|z| \to \infty$.

We begin by rewriting (4) as $h(z,\alpha) = \pi^{-1}\int_0^\infty F_\alpha(\omega)\cos(\omega z)\,\mathrm{d}\omega$, where

$$F_\alpha(\omega) := \widehat{G}(\omega)\widehat{L}(\alpha\omega) = \mathrm{e}^{\alpha^2/2}\widehat{G}(\omega+\alpha) = \frac{\widehat{G}(\omega+\alpha)}{\widehat{G}(\alpha)}.$$

Using repeated integration by parts yields

$$h(z,\alpha) = \frac{1}{\pi}\left[\sum_{k=1}^{n}\frac{(-1)^k F_\alpha^{(2k-1)}(0)}{z^{2k}} + \frac{(-1)^n}{z^{2n}}\int_0^\infty F_\alpha^{(2n)}(\omega)\cos(\omega z)\,\mathrm{d}\omega\right]. \tag{14}$$

Of course, we put

$$\overline{h}_n(z,\alpha) := \frac{1}{\pi}\sum_{k=1}^{n}\frac{(-1)^k F_\alpha^{(2k-1)}(0)}{z^{2k}}$$

and we note that

$$\begin{aligned}
F_\alpha^{(1)}(0) &= -\alpha \\
F_\alpha^{(3)}(0) &= -\alpha^3 + 3\alpha \\
F_\alpha^{(5)}(0) &= -\alpha^5 + 10\alpha^3 - 15\alpha \\
F_\alpha^{(7)}(0) &= -\alpha^7 + 21\alpha^5 - 105\alpha^3 + 105\alpha \\
F_\alpha^{(9)}(0) &= -\alpha^9 + 36\alpha^7 - 378\alpha^5 + 1260\alpha^3 - 945\alpha.
\end{aligned}$$

The general formula for $F_\alpha^{(m)}$ is obtained by noting that $(-1)^m\widehat{G}^{(m)}(\omega)/\widehat{G}(\omega)$ is the mth Hermite polynomial.

To analyse the error incurred when using the expansion, first note that by the Riemann–Lebesgue lemma, the integral in (14) goes to zero as $|z| \to \infty$. Hence, $\pi z^{2n}|h(z,\alpha)-\overline{h}_n(z,\alpha)|$ goes to zero as $|z| \to \infty$, and we have an asymptotic expansion of the Poincaré-type [2, p 15]. To analyse the asymptotic relative error, note that as $|z| \to \infty$, (14) implies $\pi z^2 h(z,\alpha) \to -F'_\alpha(0) = \alpha$, while $\pi z^2|h(z,\alpha)-\overline{h}_n(z,\alpha)|$ converges to zero. Thus, the relative error, $|h(z,\alpha)-\overline{h}_n(z,\alpha)|/|h(z,\alpha)|$ converges to zero.

Numerical bounds on the above errors can be obtained by noting that the magnitude of the integral in (14) is less than $\int_0^\infty |F_\alpha^{(2n)}(\omega)|\,\mathrm{d}\omega$, which can be computed easily with a numerical integration routine for small α and n.

Remark. After appropriate scaling, it can be seen that $\overline{h}_n$ is equivalent to [9, equation (14)]. The derivation in [9] is quite different from ours, and no error analysis is given.

Numerical example

The application that motivated this work required the computation of $h(z,\alpha)$ for all z and all $\alpha \in [0.1, 4]$. To obtain an approximation with a relative error of less than 1×10^{-6}, we proceeded as follows. Since h can be computed quite accurately, though slowly, with a numerical integration routine, we first observed that the asymptotic expansion $\overline{h}_5$ yields a relative error of less than 1×10^{-6} for $|z| > 11$ when $\alpha \in [0.1, 4]$. To approximate h for $|z| \leqslant 11$, we proceeded as follows. From the graphs of h shown in figure 1 for several values of α, we saw that the minimum value of h occurs at $z = \pm 11$ and $\alpha = 0.1$, for which $h(\pm 11, 0.1) = 2.7 \times 10^{-4}$. So, to obtain a relative error of less than 1×10^{-6}, it suffices to bound the absolute error between h and $\tilde{h}_{W,N}$ by 2.7×10^{-10}. By taking $W = 14$, we found that the bounds in (6) and (12) were 5.00×10^{-13} and 4.58×10^{-13}, respectively. By computing the integral in (11) for $n \geqslant 1$ numerically, we found that the largest magnitude for $n > N = 15$ was achieved at $n = 16$ yielding $\overline{K}_{15}(14) = 4.88 \times 10^{-10}$. Thus, the bound in (10) is 1.95×10^{-10}, and the total uniform error bound is 2.4×10^{-10} as required.

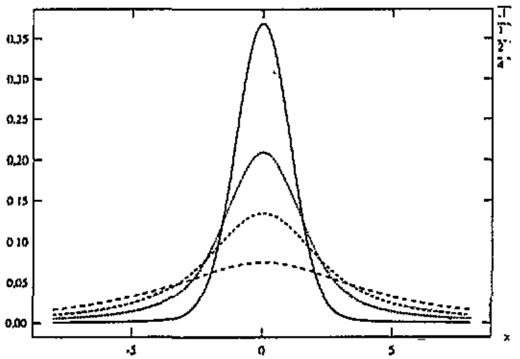

Figure 1. Graphs of $h(z,\alpha)$. The legend indicates the different values of α.

Appendix

We now establish (10). We begin with two simple observations. The first is that $\sum_{n=N+1}^{\infty} 1/n^2 \leqslant 1/N$, which follows by an integral comparison. The second observation is that since $I_n(z,\alpha,W)$ is equal to (8), $|I_n(z,\alpha,W)| \leqslant 1/\alpha_{\min}$.

The remainder of the proof consists of showing that $\hat{g}_n$ is $O(n^{-2})$. More precisely, we use a standard application of integration by parts to show that $|\hat{g}_n|$ is less than a constant divided by n^2, and we identify the constant.

Since $\widehat{G}$ is even, rewrite (7)

$$\hat{g}_n = \frac{2}{W}\int_0^{W/2} \widehat{G}(\omega)\cos(nz_0\omega)\,d\omega$$

and then integrate by parts twice and use the fact that $z_0 W = 2\pi$ and the fact that $\widehat{G}'(0) = 0$. We obtain

$$\hat{g}_n = \frac{1}{n^2 z_0^2}\left[-(-1)^n e^{-W^2/8} + 2K_n(W)/W\right]$$

where $K_n(W)$ denotes the integral in (11). This establishes (10).

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