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New Approximations to Familiar Functions

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Abstract. Using an integral representation of the Hermite polynomial and then Gaussian quadrature, very accurate representations are obtained for $\exp(-z^2)$, $\operatorname{erf}(z)$, and $\arcsin(z)$.

1. Introduction. In many areas of applied mathematics, including numerical evaluations by computer and in pharmacokinetic model building, it is useful to have accurate representations of functions in terms of sums of exponentials, sines or cosines. For example, Bellman et al. [2] recently expressed $\exp(-z^2)$ as a sum of exponentials based on differential approximations. In this paper, very accurate representations for $\exp(-z^2)$, $\operatorname{erf}(z)$ and $\arcsin(z)$ are obtained and compared to exact results for $0 \leqq z \leqq 1$. The formulas, however, are valid for all real z.

In each case, the elementary function is expressed as a Gaussian integral in which the integrand contains the function $\exp(-x^2)$ and the limits of integration are either $(0, \infty)$ or $(-\infty, \infty)$. These representations are special cases of the more general result in which Dutt [4] expressed the general multivariate normal probability integral as the sum of Fourier integral transforms involving multivariate normal characteristic functions.

2. Complete Integral Representations of $\exp(-z^2)$, $\operatorname{erf}(z)$ and $\arcsin(z)$. The tetrachoric functions $\{\tau_m(x)\}$ are defined [1, p. 934] by

$$\tau_m(x) = Z(x)He_{m-1}(x)/(m!)^{1/2}, \qquad m = 1, 2, \cdots, \tag{2.1}$$

where

$$Z(x) = (1/(2\pi)^{1/2}) \exp(-x^2/2)$$

and $He_n(x)$ is the nth degree Hermite polynomial

$$He_n(x) = (-1)^n/Z(x)\left(\frac{d}{dx}\right)^n Z(x), \qquad n = 0, 1, \cdots. \tag{2.2}$$

From the integral representation of the Hermite polynomial [1], an integral representation of the tetrachoric function $\tau_m(x)$ is obtained as

$$\tau_m(x) = (1/\pi(m!)^{1/2}) \int_0^\infty \exp(-s^2/2)s^{m-1} \cos(xs - (m - 1)\pi/2)\, ds, \qquad m = 1, 2, \cdots. \tag{2.3}$$

To obtain the integral representation for $\exp(-z^2)$, equate relations (2.1) and (2.3)

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for $m = 1$ to obtain

$$\exp(-x^2/2) = (2/\pi)^{1/2} \int_0^\infty \exp(-s^2/2) \cos xs \, ds.$$

The setting of $z = x/\sqrt{2}$ and $u = s/\sqrt{2}$ yields the desired integral expression for $\exp(-z^2)$,

$$\exp(-z^2) = (2/\sqrt{\pi}) \int_0^\infty \exp(-u^2) \cos 2zu \, du. \tag{2.4}$$

This, of course, is the well-known relation between normal probability density and characteristic function.

Next, for $\operatorname{erf}(z)$ recall first the definition [1, p. 297]

$$\operatorname{erf}(z) = (2/\sqrt{\pi}) \int_0^z \exp(-t^2) \, dt. \tag{2.5}$$

The substitution of (2.4) into the integrand of (2.5), followed by a permissible interchange of order of integration and then integration with respect to t, gives the desired complete integral form for $\operatorname{erf}(z)$,

$$\operatorname{erf}(z) = (2/\pi) \int_0^\infty \exp(-u^2) \sin 2zu \, du/u. \tag{2.6}$$

Finally, the complete integral representation for arcsin z was obtained by Childs [3] by application of Parseval's theorem and by Dutt [4] using the integral representation equation (2.3) applied to Pearson's tetrachoric series. Both approaches use the bivariate normal probability integral as the starting point.

The integral form most useful for the purposes here is

$$\arcsin z = (2/\pi) \int_0^\infty \int_0^\infty \exp(-(u^2 + v^2)) \sinh 2zuv \, du \, dv/uv. \tag{2.7}$$

3. Numerical Results. The three integrals in Eqs. (2.4), (2.6) and (2.7) are evaluated by the Gaussian quadrature formula [1, p. 924], which for an arbitrary function $f(t)$ is defined as

$$\int_{-\infty}^\infty \exp(-t^2) f(t) \, dt = \sum_{m=1}^M w_m f(x_m) + R_M, \tag{3.1}$$

where $\{w_m\}$ are the Christoffel weight factors; $\{x_m\}$ are the zeros of $He_m(x)$ and R_M, the remainder after M terms is given by

$$R_M = \pi^{1/2} f^{(2M)}(\xi)/2^M(2M)(2M-1) \cdots (M+2)(M+1), \qquad -\infty < \xi < +\infty.$$

Using Eq. (3.1) and neglecting remainder terms, the Gaussian quadrature formulas corresponding to integrals (2.4), (2.6) and (2.7) are given by

$$\exp(-z^2) = (2/\sqrt{\pi}) \sum_{i=1}^N w_i \cos(\lambda_i z\sqrt{2}), \tag{3.2}$$

$$\operatorname{erf}(z) = (2\sqrt{2}/\pi) \sum_{i=1}^N y_i \sin(\lambda_i z\sqrt{2}), \tag{3.3}$$

$$\arcsin(z) = (4/\pi) \sum_{i,j=1}^{N} y_i y_j \sinh(\lambda_i \lambda_j z), \tag{3.4}$$

respectively, where $y_i = w_i/\lambda_i$ and $\lambda_i = 2^{1/2}x_i$ for $i = 1, \cdots, N$ and $N = M/2$, which is to indicate that only positive zeros $\{x_i\}$ are necessary. It is noted that the right side of Eq. (3.4) is a symmetric quadratic form, so that computation involves $N(N+1)/2$ terms rather than N^2.

The numerical values of all three functions for $0 \leqq z \leqq 1$, along with the corresponding errors, are listed in Table 1.

TABLE I
The Calculated Values of $\exp(-z^2)$, erf(z) and arcsin(z).

	$\exp(-z^2)$			erf(z)			arcsin(z)		
z	N	eq(3.2)	$E \times 10^{-6}$	N	eq(3.3)	$E \times 10^{-6}$	N	eq(3.4)	$E \times 10^{-6}$
.1	2	0.99004983	0	2	0.11246292	0	2	0.10016742	0
.2	3	0.96078943	+.01	2	0.22270259	0	3	0.20135792	0
.3	3	0.91393118	+.01	3	0.32862676	0	3	0.30469265	0
.4	3	0.85214378	+.01	3	0.42839235	+.01	3	0.41151682	+.03
.5	3	0.77880076	+.02	3	0.52049987	+.01	4	0.52359876	+.02
.6	4	0.69767632	+.01	3	0.60385607	+.02	5	0.64350108	+.03
.7	4	0.61262639	0	4	0.67780119	0	6	0.77539746	+.04
.8	5	0.52729241	+.01	4	0.74210097	−.01	8	0.92729500	+.22
.9	5	0.44485805	+.02	4	0.79690821	0	12	1.11976780	+1.71
1.0	5	0.36787942	+.02	5	0.84270079	0	*	———	———

$E \times 10^{-6}$ = difference of the exact value minus the value calculated.
* Not feasible to use this method to calculate arcsin(z) near $z = 1$.

4. Discussion. Very accurate approximations (almost 8 significant digits) are obtained for $\exp(-z^2)$ and erf(z) in $0 \leqq z \leqq 1$, using no more than $N = 5$ terms. For arcsin(z), in general, higher values N are needed for accurate results. Indeed, this arcsin representation breaks down in the neighborhood of $z = 1$, since the value $z = 1$ corresponds to a unity correlation coefficient in the bivariate normal distribution. Such a distribution which has a singular correlation matrix is commonly termed a singular normal distribution [6].

Complete integral representations are already well known for certain other functions. The integral representation of I_n, the modified Bessel function, in $\{-1, 1\}$ can be useful to obtain approximations for the distribution of noncentral chi square. A past result involving I_0 might be of interest [5]. Complete integral representations and corresponding numerical approximations can also be obtained for the bivariate distributions of chi square and F.

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