Approximations for the $x \exp x^2$ erfc x Function

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The exp x^2 erfc x function occurs frequently in diffusion theory and in related fields. The need for an approximation to this function arose in this laboratory in connection with the on-line handling of experimental data by a small computer. The requirements for the computer routine were that the approximation should be accurate to one-tenth of a percent or better for all positive values of the argument and that the routine be simple in the following respects: occupy few memory locations, operate with few and relatively imprecise parameters, and avoid very large or very small floating point numbers. That the approximation be rational was not essential.

Though the approximations due to Hastings [1] represent the error function with small absolute error, they lead to large relative errors in the exp x^2 erfc x product at extreme values of x. Alternative approximations were therefore sought and those here proposed are inspired by the relation 7.1.13 in [2]

(1)
$$F(x) = \sqrt{\pi x} \exp x^2 \operatorname{erfc} x = \frac{2}{1 + [1 + 2x^{-2}\Phi(x)]^{1/2}}$$

which defines a slowly-varying function $\Phi(x)$ such that $\Phi(0) = 2/\pi$ and $\Phi(\infty) = 1$. So that the approximation would be exact in the limits x = 0 and $x \to \infty$

(2)
$$1 - (1 - 2/\pi) \exp\{-xP(x)\}$$

was substituted for $\Phi(x)$ and empirical methods were then used to construct simple polynomials P(x) such that F(x) reproduces tabled values of this function [2] with small relative errors. A simple polynomial,

(3)
$$P(x) = 0.845$$

gives a maximum error (near x = 2) of one part in 1200. The form a + bx offers little advantage and the most successful two-parameter expression found was the cubic

(4)
$$P(x) = a[1 - bx^2(1 - ax/\pi^2)]$$

with a = 0.8577 and b = 0.024. These values are close to "best" in the Chebyshev sense and lead to an oscillatory error curve developing a maximal relative error between the exact and the approximate F(x) of one part in 7000 close to the values x = 0.1, x = 0.7, and x = 2.0, and showing greatly enhanced agreement as the argument approaches extremely small or large values.

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