$i\operatorname{erfc} z$ and $i^2\operatorname{erfc} z$ correct to 6 significant figures (7 s.f. for $z > 1$) using single precision on a computer with word length of 8 decimal places, for all z for which e^{-z^2} can be calculated correctly. To obtain greater accuracy, it is necessary either to use double precision or to use more than two different expansions for each function. From Gautschi's formula [2] for the number of terms required for calculation by backward recurrence, we see that that method will be better (for 7 s.f. accuracy) if all the z's of interest are greater than about 2.5. The advantage accruing from the use of Chebyshev approximations would be still greater for multiple-precision calculations of very high accuracy.

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An Integral Representation for the Modified Bessel Function of the Third Kind, Computable for Large, Imaginary Order

By James D. Lear and James E. Sturm

The one-dimensional Schroedinger equation describing the quantum-mechanical motion of a particle of total energy E and mass μ in a potential field of the form:

$$V = B\exp(-r/a) \quad \text{for } r > 0$$
$$V = \infty \quad \text{for } r \leq 0$$

has, as time-independent solutions, the functions

$$\left(\frac{\nu \sinh \pi\nu}{\pi}\right)^{1/2} K_{i\nu}(z)$$

where $\nu = 2a(2\mu E/\hbar^2)^{1/2}$, $z = 2aBe^{-r/2a}$, $K_{i\nu}(z)$ is the modified Bessel function of the third kind, and the normalization is to unit amplitude of the asymptotic (r increasing) solution [1]. In attempting to compute values for $K_{i\nu}(z)$ through use of the representation:

Received April 7, 1966.

$$K_{i\nu}(z) = \int_0^\infty \exp\,[-z\cosh\phi]\cos\nu\phi d\phi \tag{1}$$

evaluated by Simpson's rule on a digital computer, we found that computational precision was quickly lost for $\nu > 15$ and ν/z around or exceeding unity. The reason for this is evident when one considers the fact that, while $K_{i\nu}(z)$ has a maximum amplitude of the order $(\pi/\nu \sinh \pi\nu)^{1/2}$, the maximum amplitude of the integrand in (1) is independent of ν. Hence, as ν increases, the accuracy requirement for the integration increases and eventually exceeds that afforded by the word sizes of most electronic computing machines. Below is given a simple generalization of (1) by which the excessive accuracy requirement can be replaced by an increase in the time required for the numerical integration.

We note that $K_{i\nu}(z)$ is a real function related to the Hankel function of the first kind via:

$$K_{i\nu}(z) = \frac{\pi}{2}\exp\,[\pi i(1 + i\nu)/2]H_{i\nu}^{(1)}(iz)\,. \tag{2}$$

Beginning with the integral representation for the Hankel function:

$$H_{i\nu}^{(1)}(iz) = \frac{1}{\pi}\int_{\text{path}} \exp\,[-z\cos\phi - \nu(\phi - \pi/2)]d\phi \tag{3}$$

where the path in the complex ϕ plane extends from $i\infty$ to $-i\infty$ within the strip $|\mathrm{Re}\,\phi| < \pi/2$, we let $w = u + iv = -i\phi$, reverse the w plane path, and multiply the resulting expression by $-(\pi/2)\exp\,[\pi i(1 + i\nu)/2]$ to obtain, considering (2):

$$K_{i\nu}(z) = \frac{1}{2}\int_{-\infty + ib}^{\infty + ia} \exp\,[-z\cosh w - i\nu w]dw\,, \qquad |a|, |b| < \pi/2\,. \tag{4}$$

With $w = u + iv$, (4) can be expressed as:

$$K_{i\nu}(z) = \frac{1}{2}\int_{-\infty + ib}^{\infty + ia} e^{\nu v}\exp\,[-z\cosh u\cos v]\cos\,(z\sinh u\sin v + \nu u)\,dw \tag{5}$$

where we have used the fact that $K_{i\nu}(z)$ is real to eliminate the imaginary part of (4). If we now let v be constant along the integration path, we obtain:

$$K_{i\nu}(z) = \int_0^\infty e^{\nu v}\,e^{-z\cosh u\cos v}\cos\,(z\sinh u\sin v + \nu u)\,du \tag{6}$$

which, for $v = 0$, reduces to the standard definition.

The advantage of (6) comes in the dependence of the integrand amplitude on v. By adjusting v to be a negative constant (greater than $-\pi/2$), the large fluctuations of the integrand can be suppressed to tolerable magnitudes. The slower convergence of (6), while not as serious a problem as the former requirement of huge word sizes, will limit the applicability of the representation to a range of ν within which error accumulation in the integration can be held within tolerable limits.

The table given below shows how the accuracy of an evaluation depends on the choice of v for constant ($\pm 1\%$) values of $\cos v \cosh B$. B is the upper limit on u in the integration and D is the size of the Simpson's rule increment in u, both parameters being chosen to give a 6-significant-figure accuracy limit for v approaching $-\pi/2$.

	Evaluation of $K_{i50}(20)$		
Value $\times 10^{34}$	v	B	D
−.723828	−1.00	3.65	.0025
.269938	−1.20	4.00	"
.274077	−1.40	4.80	"
.274078	−1.48	5.45	"
"	−1.50	5.60	.005
"	−1.52	6.00	"
"	−1.54	6.50	"

Acknowledgement. This work was supported by the Atomic Energy Commission under Contract No. AT(30-1)-2772 which included access to the CDC-6600 facility at the Courant Institute for Mathematical Sciences at New York University.

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Mixed Algebraic-Exponential Interpolation Using Finite Differences

By J. W. Layman

The use of finite differences in exponential polynomial interpolation was introduced in [1], where an algorithm was developed which triangularizes the system of equations that determines the coefficients in the interpolating exponential polynomial. In the present note we show that a similar finite-difference algorithm also exists for interpolation by a mixed algebraic-exponential polynomial of the form

$$P(x) = \sum_{n=1}^{N} \sum_{m=0}^{m_n} a_{nm} x^{(m)} n^x \tag{1}$$

for $x = 0, 1, 2, \cdots, \sum_{n=1}^{N} (m_n + 1) - 1$. The symbol $x^{(m)}$ represents the factorial power function $x(x-1)\cdots(x-m+1)$.

We require the basic difference operations E and Δ and, in addition, the diagonal difference S defined by $Sf(x) = \Delta^x f(0)$. The diagonal difference is more precisely defined in [1] and certain difficulties in interpretation are resolved there. These arise when taking higher-order diagonal differences by iteration, $S^n f(x) = SS^{n-1}f(x)$.

The following properties and formulas involving the diagonal-difference opera-

Received April 28, 1966. Revised December 5, 1966.