$i\text{erfc} z$ and $i^2 \text{erfc} z$ 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 $\mu$ in a potential field of the form:

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

has, as time-independent solutions, the functions

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

where $\nu = 2a(2\mu E/h^2)^{1/2}$, $z = 2aB e^{-r/2a}$, $K_{\nu}(z)$ 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 $K_{\nu}(z)$ through use of the representation:

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(1) 
\[ K_\nu(z) = \int_0^\infty \exp \left[ -z \cosh \phi \right] \cos \nu \phi d\phi \]
evaluated by Simpson’s rule on a digital computer, we found that computational precision was quickly lost for \( \nu > 15 \) and \( \nu/z \) around or exceeding unity. The reason for this is evident when one considers the fact that, while \( K_\nu(z) \) 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 \( \nu \). Hence, as \( \nu \) 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 \( K_\nu(z) \) is a real function related to the Hankel function of the first kind via:

(2) 
\[ K_\nu(z) = \frac{\pi}{2} \exp \left[ \frac{\pi i(1 + i\nu)/2}{2} \right] H^{(1)}_{\nu}(iz) . \]

Beginning with the integral representation for the Hankel function:

(3) 
\[ H^{(1)}_{\nu}(iz) = \frac{1}{\pi} \int_{\text{path}} \exp \left[ -z \cos \phi - \nu(\phi - \pi/2) \right] d\phi \]

where the path in the complex \( \phi \) plane extends from \( i \infty \) to \( -i \infty \) within the strip \( |\text{Re } \phi| < \pi/2 \), 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):

(4) 
\[ K_\nu(z) = \frac{1}{2} \int_{a+ia}^{a+ib} \exp \left[ -z \cosh w - iw \right] dw , \quad |a|, |b| < \pi/2 . \]

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

(5) 
\[ K_\nu(z) = \frac{1}{2} \int_{a+ia}^{a+ib} e^{zw} \exp \left[ -z \cosh u \cos v \right] \cos (z \sinh u \sin v + vu) \, dw \]

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

(6) 
\[ K_\nu(z) = \int_0^\infty e^{zw} e^{-z \cosh u \cos v} \cos (z \sinh u \sin v + vu) \, du \]

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 \( \nu \) 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 (±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 \(-\pi/2\).
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

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

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

We require the basic difference operations \( E \) and \( \Delta \) and, in addition, the diagonal difference \( S \) defined by \( Sf(x) = \Delta^2 f(0) \). 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, \( S^nf(x) = SS^{n-1}f(x) \).

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

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