Of course you should calculate repeated subexpressions, like c/d or d/c, only once.

Complex square root is even more complicated, since we must both guard intermediate results, and also enforce a chosen branch cut (here taken to be the negative real axis). To take the square root of $c + id$, first compute

$$w \equiv \begin{cases} 0 & c = d = 0 \\ \sqrt{|c|}\sqrt{\dfrac{1+\sqrt{1+(d/c)^2}}{2}} & |c| \geq |d| \\ \sqrt{|d|}\sqrt{\dfrac{|c/d|+\sqrt{1+(c/d)^2}}{2}} & |c| < |d| \end{cases} \tag{5.4.6}$$

Then the answer is

$$\sqrt{c+id} = \begin{cases} 0 & w = 0 \\ w + i\left(\dfrac{d}{2w}\right) & w \neq 0, c \geq 0 \\ \dfrac{|d|}{2w} + iw & w \neq 0, c < 0, d \geq 0 \\ \dfrac{|d|}{2w} - iw & w \neq 0, c < 0, d < 0 \end{cases} \tag{5.4.7}$$

CITED REFERENCES AND FURTHER READING:

Midy, P., and Yakovlev, Y. 1991, *Mathematics and Computers in Simulation*, vol. 33, pp. 33–49.

Knuth, D.E. 1981, *Seminumerical Algorithms*, 2nd ed., vol. 2 of *The Art of Computer Programming* (Reading, MA: Addison-Wesley) [see solutions to exercises 4.2.1.16 and 4.6.4.41].

5.5 Recurrence Relations and Clenshaw's Recurrence Formula

Many useful functions satisfy recurrence relations, e.g.,

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{5.5.1}$$

$$J_{n+1}(x) = \frac{2n}{x}J_n(x) - J_{n-1}(x) \tag{5.5.2}$$

$$nE_{n+1}(x) = e^{-x} - xE_n(x) \tag{5.5.3}$$

$$\cos n\theta = 2\cos\theta\cos(n-1)\theta - \cos(n-2)\theta \tag{5.5.4}$$

$$\sin n\theta = 2\cos\theta\sin(n-1)\theta - \sin(n-2)\theta \tag{5.5.5}$$

where the first three functions are Legendre polynomials, Bessel functions of the first kind, and exponential integrals, respectively. (For notation see [1].) These relations

are useful for extending computational methods from two successive values of n to other values, either larger or smaller.

Equations (5.5.4) and (5.5.5) motivate us to say a few words about trigonometric functions. If your program's running time is dominated by evaluating trigonometric functions, you are probably doing something wrong. Trig functions whose arguments form a linear sequence $\theta = \theta_0 + n\delta$, $n = 0, 1, 2, \ldots$, are efficiently calculated by the following recurrence,

$$\begin{aligned} \cos(\theta + \delta) &= \cos\theta - [\alpha\cos\theta + \beta\sin\theta] \\ \sin(\theta + \delta) &= \sin\theta - [\alpha\sin\theta - \beta\cos\theta] \end{aligned} \tag{5.5.6}$$

where α and β are the precomputed coefficients

$$\alpha \equiv 2\sin^2\left(\frac{\delta}{2}\right) \qquad \beta \equiv \sin\delta \tag{5.5.7}$$

The reason for doing things this way, rather than with the standard (and equivalent) identities for sums of angles, is that here α and β do not lose significance if the incremental δ is small. Likewise, the adds in equation (5.5.6) should be done in the order indicated by square brackets. We will use (5.5.6) repeatedly in Chapter 12, when we deal with Fourier transforms.

Another trick, occasionally useful, is to note that both $\sin\theta$ and $\cos\theta$ can be calculated via a single call to $\tan$:

$$t \equiv \tan\left(\frac{\theta}{2}\right) \qquad \cos\theta = \frac{1 - t^2}{1 + t^2} \qquad \sin\theta = \frac{2t}{1 + t^2} \tag{5.5.8}$$

The cost of getting both $\sin$ and $\cos$, if you need them, is thus the cost of $\tan$ plus 2 multiplies, 2 divides, and 2 adds. On machines with slow trig functions, this can be a savings. *However*, note that special treatment is required if $\theta \to \pm\pi$. And also note that many modern machines have *very fast* trig functions; so you should not assume that equation (5.5.8) is faster without testing.

Stability of Recurrences

You need to be aware that recurrence relations are not necessarily *stable* against roundoff error in the direction that you propose to go (either increasing n or decreasing n). A three-term linear recurrence relation

$$y_{n+1} + a_n y_n + b_n y_{n-1} = 0, \qquad n = 1, 2, \ldots \tag{5.5.9}$$

has two linearly independent solutions, f_n and g_n say. Only one of these corresponds to the sequence of functions f_n that you are trying to generate. The other one g_n *may* be exponentially growing in the direction that you want to go, or exponentially damped, or exponentially neutral (growing or dying as some power law, for example). If it is exponentially growing, then the recurrence relation is of little or no practical use in that direction. This is the case, e.g., for (5.5.2) in the direction of increasing n, when $x < n$. You cannot generate Bessel functions of high n by forward recurrence on (5.5.2).

To state things a bit more formally, if

$$f_n/g_n \to 0 \quad \text{as} \quad n \to \infty \tag{5.5.10}$$

then f_n is called the *minimal* solution of the recurrence relation (5.5.9). Nonminimal solutions like g_n are called *dominant* solutions. The minimal solution is unique, if it exists, but dominant solutions are not — you can add an arbitrary multiple of f_n to a given g_n. You can evaluate any dominant solution by forward recurrence, *but not the minimal solution*. (Unfortunately it is sometimes the one you want.)

Abramowitz and Stegun (in their Introduction) [1] give a list of recurrences that are stable in the increasing or decreasing directions. That list does not contain all possible formulas, of course. Given a recurrence relation for some function $f_n(x)$ you can test it yourself with about five minutes of (human) labor: For a fixed x in your range of interest, start the recurrence not with true values of $f_j(x)$ and $f_{j+1}(x)$, but (first) with the values 1 and 0, respectively, and then (second) with 0 and 1, respectively. Generate 10 or 20 terms of the recursive sequences in the direction that you want to go (increasing or decreasing from j), for each of the two starting conditions. Look at the difference between the corresponding members of the two sequences. If the differences stay of order unity (absolute value less than 10, say), then the recurrence is stable. If they increase slowly, then the recurrence may be mildly unstable but quite tolerably so. If they increase catastrophically, then there is an exponentially growing solution of the recurrence. If you know that the function that you want actually corresponds to the growing solution, then you can keep the recurrence formula anyway e.g., the case of the Bessel function $Y_n(x)$ for increasing n, see §6.5; if you don't know which solution your function corresponds to, you must at this point reject the recurrence formula. Notice that you can do this test *before* you go to the trouble of finding a numerical method for computing the two starting functions $f_j(x)$ and $f_{j+1}(x)$: stability is a property of the recurrence, not of the starting values.

An alternative heuristic procedure for testing stability is to replace the recurrence relation by a similar one that is linear with constant coefficients. For example, the relation (5.5.2) becomes

$$y_{n+1} - 2\gamma y_n + y_{n-1} = 0 \tag{5.5.11}$$

where $\gamma \equiv n/x$ is treated as a constant. You solve such recurrence relations by trying solutions of the form $y_n = a^n$. Substituting into the above recurrence gives

$$a^2 - 2\gamma a + 1 = 0 \qquad \text{or} \qquad a = \gamma \pm \sqrt{\gamma^2 - 1} \tag{5.5.12}$$

The recurrence is stable if $|a| \leq 1$ for all solutions a. This holds (as you can verify) if $|\gamma| \leq 1$ or $n \leq x$. The recurrence (5.5.2) thus cannot be used, starting with $J_0(x)$ and $J_1(x)$, to compute $J_n(x)$ for large n.

Possibly you would at this point like the security of some real theorems on this subject (although we ourselves always follow one of the heuristic procedures). Here are two theorems, due to Perron [2]:

Theorem A. If in (5.5.9) $a_n \sim an^\alpha$, $b_n \sim bn^\beta$ as $n \to \infty$, and $\beta < 2\alpha$, then

$$g_{n+1}/g_n \sim -an^\alpha, \qquad f_{n+1}/f_n \sim -(b/a)n^{\beta-\alpha} \tag{5.5.13}$$

and f_n is the minimal solution to (5.5.9).

Theorem B. Under the same conditions as Theorem A, but with $\beta = 2\alpha$, consider the *characteristic polynomial*

$$t^2 + at + b = 0 \tag{5.5.14}$$

If the roots t_1 and t_2 of (5.5.14) have distinct moduli, $|t_1| > |t_2|$ say, then

$$g_{n+1}/g_n \sim t_1 n^\alpha, \qquad f_{n+1}/f_n \sim t_2 n^\alpha \tag{5.5.15}$$

and f_n is again the minimal solution to (5.5.9). Cases other than those in these two theorems are inconclusive for the existence of minimal solutions. (For more on the stability of recurrences, see [3].)

How do you proceed if the solution that you desire *is* the minimal solution? The answer lies in that old aphorism, that every cloud has a silver lining: If a recurrence relation is catastrophically unstable in one direction, then that (undesired) solution will decrease very rapidly in the reverse direction. This means that you can start with *any* seed values for the consecutive f_j and f_{j+1} and (when you have gone enough steps in the stable direction) you will converge to the sequence of functions that you want, times an unknown normalization factor. If there is some other way to normalize the sequence (e.g., by a formula for the sum of the f_n's), then this can be a practical means of function evaluation. The method is called *Miller's algorithm*. An example often given [1,4] uses equation (5.5.2) in just this way, along with the normalization formula

$$1 = J_0(x) + 2J_2(x) + 2J_4(x) + 2J_6(x) + \cdots \tag{5.5.16}$$

Incidentally, there is an important relation between three-term recurrence relations and *continued fractions*. Rewrite the recurrence relation (5.5.9) as

$$\frac{y_n}{y_{n-1}} = -\frac{b_n}{a_n + y_{n+1}/y_n} \tag{5.5.17}$$

Iterating this equation, starting with n, gives

$$\frac{y_n}{y_{n-1}} = -\frac{b_n}{a_n -}\,\frac{b_{n+1}}{a_{n+1} -} \cdots \tag{5.5.18}$$

Pincherle's Theorem [2] tells us that (5.5.18) converges if and only if (5.5.9) has a minimal solution f_n, in which case it converges to f_n/f_{n-1}. This result, usually for the case $n = 1$ and combined with some way to determine f_0, underlies many of the practical methods for computing special functions that we give in the next chapter.

Clenshaw's Recurrence Formula

Clenshaw's recurrence formula [5] is an elegant and efficient way to evaluate a sum of coefficients times functions that obey a recurrence formula, e.g.,

$$f(\theta) = \sum_{k=0}^{N} c_k \cos k\theta \qquad \text{or} \qquad f(x) = \sum_{k=0}^{N} c_k P_k(x)$$

Here is how it works: Suppose that the desired sum is

$$f(x) = \sum_{k=0}^{N} c_k F_k(x) \tag{5.5.19}$$

and that F_k obeys the recurrence relation

$$F_{n+1}(x) = \alpha(n,x)F_n(x) + \beta(n,x)F_{n-1}(x) \tag{5.5.20}$$

for some functions $\alpha(n,x)$ and $\beta(n,x)$. Now define the quantities y_k $(k = N, N-1, \ldots, 1)$ by the following recurrence:

$$\begin{aligned} y_{N+2} &= y_{N+1} = 0 \\ y_k &= \alpha(k,x)y_{k+1} + \beta(k+1,x)y_{k+2} + c_k \quad (k = N, N-1, \ldots, 1) \end{aligned} \tag{5.5.21}$$

If you solve equation (5.5.21) for c_k on the left, and then write out explicitly the sum (5.5.19), it will look (in part) like this:

$$\begin{aligned} f(x) = & \cdots \\ & + [y_8 - \alpha(8,x)y_9 - \beta(9,x)y_{10}]F_8(x) \\ & + [y_7 - \alpha(7,x)y_8 - \beta(8,x)y_9]F_7(x) \\ & + [y_6 - \alpha(6,x)y_7 - \beta(7,x)y_8]F_6(x) \\ & + [y_5 - \alpha(5,x)y_6 - \beta(6,x)y_7]F_5(x) \\ & + \cdots \\ & + [y_2 - \alpha(2,x)y_3 - \beta(3,x)y_4]F_2(x) \\ & + [y_1 - \alpha(1,x)y_2 - \beta(2,x)y_3]F_1(x) \\ & + [c_0 + \beta(1,x)y_2 - \beta(1,x)y_2]F_0(x) \end{aligned} \tag{5.5.22}$$

Notice that we have added and subtracted $\beta(1,x)y_2$ in the last line. If you examine the terms containing a factor of y_8 in (5.5.22), you will find that they sum to zero as a consequence of the recurrence relation (5.5.20); similarly all the other y_k's down through y_2. The only surviving terms in (5.5.22) are

$$f(x) = \beta(1,x)F_0(x)y_2 + F_1(x)y_1 + F_0(x)c_0 \tag{5.5.23}$$

Equations (5.5.21) and (5.5.23) are *Clenshaw's recurrence formula* for doing the sum (5.5.19): You make one pass down through the y_k's using (5.5.21); when you have reached y_2 and y_1 you apply (5.5.23) to get the desired answer.

Clenshaw's recurrence as written above incorporates the coefficients c_k in a downward order, with k decreasing. At each stage, the effect of all previous c_k's is "remembered" as two coefficients which multiply the functions F_{k+1} and F_k (ultimately F_0 and F_1). If the functions F_k are small when k is large, *and* if the coefficients c_k are small when k is *small*, then the sum can be dominated by small F_k's. In this case the remembered coefficients will involve a delicate cancellation and there can be a catastrophic loss of significance. An example would be to sum the trivial series

$$J_{15}(1) = 0 \times J_0(1) + 0 \times J_1(1) + \ldots + 0 \times J_{14}(1) + 1 \times J_{15}(1) \tag{5.5.24}$$

Here J_{15}, which is tiny, ends up represented as a canceling linear combination of J_0 and J_1, which are of order unity.

The solution in such cases is to use an alternative Clenshaw recurrence that incorporates c_k's in an upward direction. The relevant equations are

$$y_{-2} = y_{-1} = 0 \tag{5.5.25}$$

$$y_k = \frac{1}{\beta(k+1,x)}[y_{k-2} - \alpha(k,x)y_{k-1} - c_k], \qquad (k = 0, 1, \ldots, N-1) \tag{5.5.26}$$

$$f(x) = c_N F_N(x) - \beta(N,x)F_{N-1}(x)y_{N-1} - F_N(x)y_{N-2} \tag{5.5.27}$$

The rare case where equations (5.5.25)–(5.5.27) should be used instead of equations (5.5.21) and (5.5.23) can be detected automatically by testing whether the operands in the first sum in (5.5.23) are opposite in sign and nearly equal in magnitude. Other than in this special case, Clenshaw's recurrence is always stable, independent of whether the recurrence for the functions F_k is stable in the upward or downward direction.

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Dahlquist, G., and Bjorck, A. 1974, *Numerical Methods* (Englewood Cliffs, NJ: Prentice-Hall), §4.4.3, p. 111.

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5.6 Quadratic and Cubic Equations

The roots of simple algebraic equations can be viewed as being functions of the equations' coefficients. We are taught these functions in elementary algebra. Yet, surprisingly many people don't know the right way to solve a quadratic equation with two real roots, or to obtain the roots of a cubic equation.

There are two ways to write the solution of the *quadratic equation*

$$ax^2 + bx + c = 0 \tag{5.6.1}$$

with real coefficients a, b, c, namely

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{5.6.2}$$

and

$$x = \frac{2c}{-b \pm \sqrt{b^2 - 4ac}} \tag{5.6.3}$$

If you use *either* (5.6.2) *or* (5.6.3) to get the two roots, you are asking for trouble: If either a or c (or both) are small, then one of the roots will involve the subtraction of b from a very nearly equal quantity (the discriminant); you will get that root very inaccurately. The correct way to compute the roots is

$$q \equiv -\frac{1}{2}\left[b + \mathrm{sgn}(b)\sqrt{b^2 - 4ac}\right] \tag{5.6.4}$$

Then the two roots are

$$x_1 = \frac{q}{a} \qquad \text{and} \qquad x_2 = \frac{c}{q} \tag{5.6.5}$$

If the coefficients a, b, c, are complex rather than real, then the above formulas still hold, except that in equation (5.6.4) the sign of the square root should be chosen so as to make

$$\mathrm{Re}(b^*\sqrt{b^2 - 4ac}) \geq 0 \tag{5.6.6}$$

where Re denotes the real part and asterisk denotes complex conjugation.

Apropos of quadratic equations, this seems a convenient place to recall that the inverse hyperbolic functions $\sinh^{-1}$ and $\cosh^{-1}$ are in fact just logarithms of solutions to such equations,

$$\sinh^{-1}(x) = \quad \ln\left(x + \sqrt{x^2 + 1}\right) \tag{5.6.7}$$

$$\cosh^{-1}(x) = \pm \ln\left(x + \sqrt{x^2 - 1}\right) \tag{5.6.8}$$

Equation (5.6.7) is numerically robust for $x \geq 0$. For negative x, use the symmetry $\sinh^{-1}(-x) = -\sinh^{-1}(x)$. Equation (5.6.8) is of course valid only for $x \geq 1$. Since `FORTRAN` mysteriously omits the inverse hyperbolic functions from its list of intrinsic functions, equations (5.6.7)–(5.6.8) are sometimes quite essential.