Iterated Square Root Expansions for the Inverse Cosine and Inverse Hyperbolic Cosine

By Henry C. Thacher, Jr.

Abstract. Let \( R_1 = \sqrt{2 + 2x}, \ R_{k+1} = \sqrt{2 + R_k} \). Then \( 2^k \sqrt{|2 - R_k|} \) and \( 2^{|k|} \left| \sqrt{6 - 2 \sqrt{3 + 3R_k}} \right|^{1/2} \) both converge to \( \arccos x \) if \( |x| \leq 1 \) and to \( \text{arccosh} \ x \) if \( 1 \leq x < \infty \). Truncation errors for the two expressions are of the order of \( 2^{-2k} \) and \( 2^{-4k} \), respectively.

1. Introduction. The availability on several modern automatic computers of square root operations which are approximately as fast as multiplication or division encourages investigation as to the uses which may be made of this operation in computation. Hammer [1] has described an iterative procedure based on square roots for finding cube and other odd roots which converge more rapidly than the customary iterations, but very few other authors appear to have considered this problem. It is the purpose of this contribution to describe a set of rapidly converging square root expansions for the inverse cosine, inverse hyperbolic cosine, and hence for the natural logarithm.

2. Derivation. We start from the familiar identity

\[
\phi(x) = 2\phi\left(\frac{x}{2}\sqrt{2 + 2x}\right)
\]

where \( \phi(x) \) denotes either \( \arccos x \) \((-1 \leq x \leq 1) \) or \( \text{arccosh} \ x \) \((1 \leq x < \infty) \). We restrict the multiple-valued inverse cosine to the branch \((0 \leq \arccos x \leq \pi)\), the inverse hyperbolic cosine to the positive branch \((0 \leq \text{arccosh} \ x)\), and take all square roots positive. Applying (1) repeatedly, we have

\[
\phi(x) = 2\left(2\phi\left(\frac{1}{2}\left[2 + \sqrt{2 + 2x}\right]^{1/2}\right)\right) = 2^2\phi\left(\frac{1}{2}\left[2 + \sqrt{2 + 2x}\right]^{1/2}\right)
\]

and, after \( k \) applications,

\[
\phi(x) = 2^k\phi\left(\frac{1}{2}\left[2 + \left[2 + \cdots + \sqrt{2 + 2x}\right]^{1/2}\right]^{1/2}\right) = 2^k\phi\left(\frac{1}{2}R_k\right)
\]

where \( R_k \) contains \( k \) square roots.

We may observe that \( R_k \) is an increasing function of \( x \), and that for \( x = 1 \), the innermost square root becomes equal to \( \sqrt{2} \), so that for any \( k \),

\[
\sqrt{2} \leq R_k(x) \leq 2 \quad (-1 \leq x \leq 1)
\]

and

\[
2 \leq R_k(x) \quad (1 \leq x < \infty).
\]

Furthermore, since for \(-1 \leq x \leq 1\), \( \sqrt{2 + 2x} \geq 2x \) while the contrary is true for \( x > 1 \), \( R_k(x) \) is an increasing function of \( k \) for \(|x| < 1\), and a decreasing function of \( k \) for \( x > 1 \), and thus approaches 2 as \( k \) increases. Although we have only

\[\text{Received July 1, 1960; revised April 17, 1961. The work on this paper was supported by the U. S. Atomic Energy Commission.}\]
proved this limit for real \( x > -1 \), it can be shown to be true for all finite real or complex \( x \).

If we multiply both sides of (4) by \( 2^{-k} \), and take the cosine or hyperbolic cosine, we find

\[
\phi^{-1}(2^{-k}\phi(x)) = \frac{1}{2} R_k.
\]  

(7)

Now both the cosine and the hyperbolic cosine may be expanded in Taylor's series. If we use only the first two terms of the series, and the error term, \( E_3 \), we find

\[
1 \pm \frac{(2^{-k}\phi(x))^2}{2} + E_3 = \frac{1}{2} R_k
\]  

(8)

where the upper sign is to be used for the inverse cosine. If we use the first three terms, we have

\[
1 + \frac{(2^{-k}\phi(x))^2}{2} + \frac{(2^{-k}\phi(x))^4}{24} + E_5 = \frac{1}{2} R_k.
\]  

(9)

Solving (8) for \( \phi(x) \), remembering (5), (6), and our restrictions of the values of \( \phi \) to positive quantities, we find

\[
\phi(x) = 2^k \sqrt{2 - R_k + 2E_3}.
\]  

(10)

Equation (9), a quadratic in \( (2^{-k}\phi(x))^2 \), has the root

\[
(2^{-k}\phi(x))^2 = \left| 6 - 2 \sqrt{3 + 3R_k - 6E_5} \right|.
\]  

(11)

The second root is easily seen to give a value for \( \phi \) outside the specified range. (For \( x \leq 1 \), \( 2^{2k}(6 + 2\sqrt{3 + 3R_k - 6E_5}) > 2^{2k}(6 + 2\{3 + 3\sqrt{2}\})^{1/3} > 2^{2k} \pi^2 \), while for \( x < 1 \), \( -6 - 2\sqrt{3 + 3R_k - 6E_5} < 0 \)). Hence,

\[
\phi(x) = 2^k \{\left| 6 - 2 \sqrt{3 + 3R_k - 6E_5} \right|^{1/2} \}
\]  

(12)

The desired approximations are, of course, (10) and (12) with the error terms \( E_3 \) and \( E_5 \) omitted.

3. Truncation Error. Inverse Cosine. In estimating the truncation error incurred by neglecting \( E_3 \) or \( E_5 \), it is more convenient to analyze the expansions for \( \arccos x \) and \( \text{arccosh} x \) separately. For \( |x| \leq 1 \), (10) becomes

\[
\arccos x = 2^k \sqrt{2 - R_k + 2E_3} = 2^k \sqrt{2 - R_k} + \eta_3
\]  

(13)

while (12) becomes

\[
\arccos x = 2^k \{6 - 2 \sqrt{3 + 3R_k - 6E_5}\}^{1/2} = 2^k \{6 - 2 \sqrt{3 + 3R_k}^{1/2}\} + \eta_5.
\]  

(14)

By Taylor's theorem, expanding (13) in powers of \( E_3 \),

\[
\arccos x = 2^k \{\sqrt{2 - R_k} + 1/\sqrt{2 - R_k} + 2\theta E_3 + E_3\} \quad (0 \leq \theta \leq 1).
\]  

(15)

Now the error in the cosine expansion (8) is of the same sign as, and less in magnitude than the first neglected term, so that

\[
0 \leq E_3 \leq \frac{(2^{-k}\arccos x)^4}{24}
\]  

(16)
Hence,
\begin{align}
1/2 \sqrt{2 - R_k} &\geq 1/2 \sqrt{2 - R_k} + 2\theta E_3 \\
\text{and}
0 &\leq \eta_2 \leq 2^{-2k}(\arccos x)^4/24\sqrt{2 - R_k}
\end{align}
and the upper bound on \( \eta_2 \) is of the order of \( 2^{-2k}(\arccos x)^2 \). Expanding (14) in the same way, we find
\begin{align*}
\arccos x &= 2^k \left\{ \frac{6 - 2\sqrt{3 + 3R_k}}{2\sqrt{2 - R_k}} \right\}^{1/2} \\
+ 3E_3/\left[ \sqrt{3 + 3R_k - 6\theta E_3} \left\{ 6 - 2\sqrt{3 + 3R_k - 6\theta E_3} \right\}^{1/2} \right] \\
&\quad \left( 0 < \theta < 1 \right)
\end{align*}
while
\begin{align}
0 &\geq E_3 \geq - \frac{(2^{-k} \arccos x)^6}{720} \\
\text{so that}
0 &\geq \eta_3 \geq - \frac{2^{-4k}(\arccos x)^6}{240 \sqrt{3 + 3R_k}}
\end{align}
and \( \eta_3 \) is of the order of \( 2^{-4k} \).

Thus, our two approximations have errors of opposite sign, and provide bounds on the true value.

4. Truncation Error. Inverse Hyperbolic Cosine. For the inverse hyperbolic cosine, \( x \geq 1 \), and we have:
\begin{align}
\arccosh x &= \ln \left( x + \sqrt{x^2 - 1} \right) = 2^k \sqrt{R_k - 2 - 2E_3} = 2^k \sqrt{R_k - 2} + \eta_4 \\
\text{and}
\arccosh x &= 2^k \left\{ 2\sqrt{3 + 3R_k - 6E_3} - 6 \right\}^{1/2} = 2^k \left\{ 2\sqrt{3 + 3R_k - 6} \right\}^{1/2} + \eta_5
\end{align}
Again using Taylor's theorem,
\begin{align}
2^k \sqrt{R_k - 2 - 2E_3} = 2^k \left\{ \frac{2E_3}{2 \sqrt{R_k - 2 - \theta E_3}} \right\} \\
\left( 0 \leq \theta \leq 1 \right)
\end{align}
The remainder in the hyperbolic cosine series is
\begin{align}
E_3 &= \cosh \left( 2^{-k} \theta' \arccosh x \right) \frac{(2^{-k} \arccosh x)^4}{4!} \\
\left( 0 \leq \theta' \leq 1 \right)
\end{align}
and has bounds
\begin{align}
0 &\leq E_3 \leq \frac{\cosh \left( 2^{-k} \arccosh x \right) (2^{-k} \arccosh x)^4}{24}
\end{align}
so that
\begin{align}
\eta_3 &= - \frac{2^k E_3}{\sqrt{R_k - 2 - \theta E_3}} \geq \frac{2^k E_3}{\sqrt{R_k - 2 - E_3}} = - \frac{2^k E_3}{2^{-k} \arccosh x}
\end{align}
Hence, \( \eta_3 \) has the bounds,

\[
(28) \quad 0 \geq \eta_3 \geq -\frac{2^{-2k}(\text{arccosh} \, x)^3}{24} \cosh (2^{-k} \text{arccosh} \, x) = -\frac{2^{-2k} R_k (\text{arccosh} \, x)^3}{48}.
\]

In similar fashion

\[
(29) \quad \eta_5 = -2^k \frac{3E_5}{\left[2 \sqrt{3} + 3R_k - 6\theta E_5 - 6\right]^{1/2} \sqrt{3} + 3R_k - 6E_5}
\]

\[
(30) \quad \geq -2^k \frac{3E_5}{\left[2 \sqrt{3} + 3R_k - 6\theta E_5 - 6\right]^{1/2} \sqrt{3} + 3R_k - 6E_5} = -\frac{2^k \theta E_5}{(2^{-k} \text{arccosh} \, x) [6 + (2^{-k} \text{arccosh} \, x)^2]}.
\]

The remainder \( E_5 \) is given by

\[
(31) \quad E_5 = \cosh (2^{-k} \theta' \text{arccosh} \, x) \frac{(2^{-k} \text{arccosh} \, x)^6}{6!} \quad (0 \leq \theta' \leq 1)
\]

so that

\[
(32) \quad 0 \leq E_5 \leq \frac{\cosh (2^{-k} \text{arccosh} \, x)}{720} (2^{-k} \text{arccosh} \, x)^6
\]

and

\[
(33) \quad 0 \geq \eta_5 \geq -\frac{\cosh (2^{-k} \text{arccosh} \, x)}{120} \frac{2^{-4k} (\text{arccosh} \, x)^5}{[6 + (2^{-k} \text{arccosh} \, x)^2]} = -\frac{2^{-4k} R_k}{6 + (2^{-k} \text{arccosh} \, x)^2} (\text{arccosh} \, x)^5
\]

The error bounds given do not appear to be unduly conservative, and are approached by the actual error as \( k \) increases.

5. Roundoff Errors. These algorithms are subject to serious roundoff error when \( k \) is large, and, except for special cases (e.g. \( x = 1 \)) are incapable of evaluating the functions to the full accuracy of the arithmetic being used. This is so with either fixed or floating arithmetic, since for both algorithms, \( 2^{-2k} \phi^2(x) \), a relatively small quantity, must be calculated from the difference of two quantities which are each greater than one. Actual computing trials have indicated, however, that approximately three-quarters of the total number of digits carried may be obtained correctly, even when particular attention is not devoted to minimizing roundoff.

6. Discussion. The algorithms have three major advantages: (a) they are simple to program (and rapid to calculate when automatic square root operations are available); (b) they require only one or three stored constants; and (c) they have an extremely wide range of acceptable convergence. As can be seen from the error bounds, these expansions converge over the entire range \(-1 \leq x < \infty\), and the convergence especially for (14) and (23) is notably rapid compared to the power series. For example, using a programmed 16-significant-decimal digit double precision
interpretive routine for the LGP-30, and (23), \( \text{arccosh} \ 250.001 \) (i.e. \( \ln 500 \)) was
found correct to 4 decimal places with \( k = 5 \) (6 square roots) and to 11 places with
\( k = 10 \) (11 square roots).

The convergence of the sequence of approximations is only first order. At some
cost in programming effort, it would be clearly possible to increase the convergence
by one of the standard extrapolation techniques for accelerating the approach to
the limit. However, the excellent convergence already present makes it unlikely
that this device would be worthwhile unless the need for high accuracy was such
that it was essential to keep \( k \) as low as possible.

A special case of (13), with \( x = -1 \), has been known for a long time. This
expansion, which has the limit \( \pi \), can be obtained as one-half the perimeter of a
2\(^n\)-gon inscribed in a circle of unit radius \([2]\). However, the general case, and the
expansions obtainable by retaining the fourth-degree terms in the series for \( \cos x \)
and \( \cosh x \) appear to be new.

An Eigenvalue Problem Arising In Mass And
Heat Transfer Studies

By J. S. Dranoff

1. Introduction. In a recent paper [1], S. Katz has considered the problem of
catalytic chemical reactions occurring on the inside surface of a cylindrical tube.
For the case of laminar flow of reactant through such a tube, he has shown how one
may generate basic kinetic data for the reaction in question from easily made over-
all conversion measurements. The interested reader is referred to the original paper
for the details of this analysis and its application.

In order to make use of Katz’s analysis, one must have on hand the solution to
the following Sturm-Liouville type eigenvalue problem:

\[
\frac{d}{dx} \left( x \frac{d\phi_n(x)}{dx} \right) + \lambda_n 4x(1 - x^2)\phi_n(x) = 0, \quad 0 \leq x \leq 1
\]

\[
\phi_n(x) \quad \text{regular at} \quad x = 0 \\
\phi_n'(1) = 0
\]

where the \( \phi_n(x) \) are the eigensolutions and the \( \lambda_n \) are the eigenvalues, with \( n = 0, 1, 2, \cdots \). The first boundary condition leads, as in the case of Bessel’s functions,
to the condition \( \phi_n'(0) = 0 \).

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