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HAL Id: ensl-01780265
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Submitted on 27 Apr 2018

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On the relative error of computing complex square roots in floating-point arithmetic

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Abstract—We study the accuracy of a classical approach to computing complex square-roots in floating-point arithmetic. Our analyses are done in binary floating-point arithmetic in precision $p$, and we assume that the (real) arithmetic operations $\bigoplus, \neg, \times, \div, \sqrt{}$ are rounded to nearest, so the unit roundoff is $u = 2^{-p}$. We show that in the absence of underflow and overflow, the componentwise and normwise relative errors of this approach are at most $\frac{1}{2}u$ and $\frac{\sqrt{2}u}{2}$, respectively, and this without having to neglect terms of higher order in $u$. We then provide some input examples showing that these bounds are reasonably sharp for the three basic binary interchange formats (binary32, binary64, and binary128) of the IEEE 754 standard for floating-point arithmetic.

Index Terms—binary floating-point arithmetic; rounding error analysis; relative error; complex square root

I. INTRODUCTION

We consider the problem of computing a square root of a complex number $a + ib$ accurately in floating-point arithmetic: given two floating-point numbers $a$ and $b$, we want to deduce very good floating-point approximations to some reals $x$ and $y$ such that

$$(x + iy)^2 = a + ib. \quad (1)$$

In exact arithmetic, explicit formulas for $x$ and $y$ are easy to derive: first, by rewriting (1) as

$$x^2 - y^2 = a \quad \text{and} \quad 2xy = b,$$

and solving quadratic equations in $x^2 \geq 0$ or $y^2 \geq 0$, we obtain

$$x = \pm \sqrt{\frac{h + a}{2}}, \quad \text{and} \quad h := \sqrt{a^2 + b^2}; \quad (2)$$

and

$$y = \pm \sqrt{\frac{h - a}{2}}. \quad (3)$$

Then it suffices to adjust the signs of $x$ and $y$ in order to ensure that $2xy = b$ holds and to make the complex square root a single-valued function. For example, one can take $x \geq 0$ and $\text{sign}(y) = \text{sign}(b)$ with $\text{sign}(0) = +1$; see [2, §4.2]. (See also [4, p. 201] for a sign function supporting signed zeros.)

In floating-point arithmetic, however, it is in general not recommended to use the above formulas for $x$ and $y$ simultaneously when $b^2 < a^2$, since then cancellation can occur either when evaluating $h + a$ if $a < 0$, or when evaluating $h - a$ if $a > 0$.

To avoid such a possible loss of accuracy, Friedland [1] proposed the following approach (which is now classical and can also be seen in [4] and [2]):

- if $a \geq 0$, then compute $x$ using (2) and deduce $y$ using

  $$y = \frac{b}{2x};$$

- if $a < 0$, then compute $y$ using (3) and deduce $x$ using

  $$x = \frac{b}{2y}.$$

Note that in the above expressions division by zero can be avoided by assuming that $(a, b) \neq (0, 0)$ and by handling the situation where $a = b = 0$ separately.

Since $h - a = h + |a|$ when $a < 0$, we see that the two cases in Friedland’s approach eventually rely on a single core computation, which can be summarized as follows: given two floating-point numbers $a$ and $b$ such that

$$(a, b) \neq (0, 0) \quad \text{and} \quad a \geq 0,$$

evaluate

$$h = \sqrt{a^2 + b^2}, \quad x = \sqrt{\frac{h + a}{2}}, \quad y = \frac{b}{2x}.$$

In radix-2, precision-$p$ floating-point arithmetic with rounding to nearest (RN), this corresponds to Algorithm 1 below.

Algorithm 1 Core computation of $\sqrt{a + ib}$, assuming $(a, b) \neq (0, 0)$ and $a \geq 0$.  

1: $s_a \leftarrow \text{RN}(a^2)$  
2: $s_b \leftarrow \text{RN}(b^2)$  
3: $s \leftarrow \text{RN}(s_a + s_b)$  
4: $\rho \leftarrow \text{RN}(\sqrt{s})$  
5: $\nu \leftarrow \text{RN}(\rho + a)$  
6: $\bar{x} \leftarrow \text{RN}(\sqrt{\nu/2})$  
7: $\bar{y} \leftarrow \text{RN}(b/(2\bar{x}))$

A detailed rounding error analysis of Algorithm 1 is given by Hull, Fairgrieve, and Tang in [2]: assuming that
underflows and overflows do not occur and using the fact that for any real number \( t \),
\[
\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq u := 2^{-p}, \tag{4}
\]
they show that the computed floating-point numbers \( \hat{x} \) and \( \hat{y} \) satisfy
\[
\frac{|\hat{x} - x|}{|x|} \leq \frac{5}{2} u + O(u^2)
\]
and
\[
\frac{|\hat{y} - y|}{|y|} \leq \frac{7}{2} u + O(u^2);
\]
they also show that for \( \hat{x} = \hat{x} + i\hat{y} \) and \( z = x + iy \), the associated normwise relative error \( |\hat{z} - z|/|z| \) admits a bound smaller than \( \frac{3}{2} u + O(u^2) \), namely,
\[
\frac{|\hat{z} - z|}{|z|} \leq \frac{\sqrt{37}}{2} u + O(u^2), \quad \frac{\sqrt{37}}{2} = 3.041 \ldots
\]
Finally, for the binary32 format \( (p = 24) \), they provide two numbers \( a \) and \( b \) for which \( |\hat{z} - z|/|z| \approx 2.980u \).

In this paper, we refine the analysis of \([2]\) in two ways: we show that the terms \( O(u^2) \) in the three bounds above can be removed and, on the other hand, we give examples of inputs in the binary64 and binary128 formats (that is, for \( p = 53 \) and \( p = 113 \)) for which \( |\hat{z} - z|/|z| > 3u \).

For our analyses it will be useful to exploit the following refinement of \((4)\), which can be found for example in \([5, p. 232]\):
\[
\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq \frac{u}{1 + u}. \tag{5}
\]
We shall apply \((5)\) to floating-point additions and multiplications; for floating-point divisions and square roots, we can use the following smaller bounds, introduced in \([3]\). Let \( a \) and \( b \) be two floating-point numbers. If \( a \geq 0 \), then
\[
\text{RN}(\sqrt{a}) = \sqrt{a} (1 + \delta), \quad |\delta| \leq 1 - \frac{1}{\sqrt{1 + 2u}}; \tag{6}
\]
if \( b \neq 0 \), then
\[
\text{RN}\left(\frac{a}{b}\right) = \frac{a}{b} (1 + \delta), \quad |\delta| \leq u - 2u^2. \tag{7}
\]
As we shall see in \[\text{III}\], the bounds in \((5-7)\) are enough to show that \( |\hat{x} - x| \leq \frac{5}{2} u|x| \). However, our analysis for \( \hat{y} \) will use some variants of \((6)\) and \((7)\), which we detail in \[\text{III}\]. We conclude in \[\text{IV}\] with the derivation of the normwise bound and three numerical examples.

II. REFINING THE BOUND ON \(|\hat{x} - x|/|x|\]

First, let us apply \((5)\) to steps 1, 2, 3 of Algorithm 1: we have
\[
(a^2) \left(1 - \frac{u}{1 + u}\right) \leq s_a = a^2 \left(1 + \frac{u}{1 + u}\right)
\]
and similarly for \( s_b \), so that
\[
(a^2 + b^2) \left(1 - \frac{u}{1 + u}\right) \leq s_a + s_b \leq (a^2 + b^2) \left(1 + \frac{u}{1 + u}\right)
\]
and then
\[
(a^2 + b^2) \left(1 - \frac{u}{1 + u}\right)^2 \leq s \leq (a^2 + b^2) \left(1 + \frac{u}{1 + u}\right)^2.
\]
By taking square roots and with \( h = \sqrt{a^2 + b^2} \), we find
\[
h \left(1 - \frac{u}{1 + u}\right) \leq \sqrt{s} \leq h \left(1 + \frac{u}{1 + u}\right).
\]
Using \((6)\), we deduce that the value of \( \rho = \text{RN}(\sqrt{s}) \) at step 4 of Algorithm 1 satisfies
\[
hL \leq \rho \leq hU,
\]
where
\[
L := \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{\sqrt{1 + 2u}} = 1 - 2u + \frac{7}{2} u^2 + O(u^3)
\]
and
\[
U := \left(1 + \frac{u}{1 + u}\right) \left(2 - \frac{1}{\sqrt{1 + 2u}}\right) = 1 + 2u - \frac{3}{2} u^2 + O(u^3).
\]
Since \( a \geq 0 \) and \( 0 \leq L \leq 1 \leq U \), this leads to
\[
(h + a)L \leq \rho + a \leq (h + a)U.
\]
By applying \((5)\), we see that \( \nu = \text{RN}(\rho + a) \) at step 5 satisfies
\[
(h + a) \left(1 - \frac{u}{1 + u}\right)^2 \cdot \frac{1}{\sqrt{1 + 2u}} \leq \nu \leq (h + a) \left(1 + \frac{u}{1 + u}\right)^2 \left(2 - \frac{1}{\sqrt{1 + 2u}}\right).
\]
Recalling that \( x = \sqrt{(h + a)/2} \), it follows that \( \sqrt{\nu/2} \) satisfies
\[
x \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{(1 + 2u)^{1/4}} \leq \sqrt{\nu/2} \leq x \left(1 + \frac{u}{1 + u}\right) \left(2 - \frac{1}{\sqrt{1 + 2u}}\right)^{1/2}.
\]
By applying \((6)\) once again, we find that the value \( \hat{x} = \text{RN}(\sqrt{\nu/2}) \) produced at step 6 satisfies
\[
xL' \leq \hat{x} \leq xU',
\]
where
\[
L' := \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{(1 + 2u)^{3/4}} = 1 - \frac{5}{2} u + \frac{41}{8} u^2 + O(u^3)
\]
and
\[
U' := \left(1 + \frac{u}{1 + u}\right) \left(2 - \frac{1}{\sqrt{1 + 2u}}\right)^{3/2} = 1 + \frac{5}{2} u - \frac{11}{8} u^2 + O(u^3).
\]
Since \( L' \geq 1 - \frac{5}{2} u \) and \( U' \leq 1 + \frac{3}{2} u \), we conclude that
\[
|\hat{x} - x| \leq \frac{5}{2} u|x|.
\]
III. REFINING THE BOUND ON $|\hat{y} - y|/|y|$

Let us now analyze the relative accuracy of the value
\[ \hat{y} = \text{RN}(b/(2x)) \]
produced by the last step of Algorithm 1. Recalling that \( y = b/(2x) \), we deduce from the bounds on \( \hat{x} \) in (8) that
\[
\frac{y}{U} \leq \frac{b}{2x} \leq \frac{y}{L'}.
\]
Applying (7) then shows that \( \hat{y} \) satisfies
\[
y \cdot \frac{1 - u + 2a^2}{U'} \leq \hat{y} \leq y \cdot \frac{1 + u - 2a^2}{L'}.
\]
One has
\[
\frac{1 - u + 2a^2}{U'} = 1 - \frac{7}{2} u + \frac{97}{8} u^2 + O(u^3)
\]
and one can check that this is larger than \( 1 - \frac{7}{2} u \).
However, the upper bound has the form
\[
\frac{1 + u - 2a^2}{L'} = 1 + \frac{7}{2} u + \frac{13}{8} u^2 + O(u^3)
\]
and is not smaller than \( 1 + \frac{7}{2} u \). Thus, at this stage, all we have is
\[
y \left( 1 - \frac{7}{2} u \right) \leq \hat{y} \leq y \left( 1 + \frac{7}{2} u + O(u^2) \right).
\]
(12)

To remove the term \( O(u^2) \), we introduce the following two lemmas, which show that the bounds in (6) and (7) can be reduced slightly under suitable assumptions.

Lemma III.1. Let \( a \) be a nonnegative floating-point number. If \( a \) is not an integral power of 2, then
\[
\text{RN}(\sqrt{a}) = \sqrt{a} (1 + \delta), \quad |\delta| \leq \frac{u}{\sqrt{1 + 6u}}.
\]
Proof. The result is clear for \( a = 0 \), so we assume that \( a > 0 \). Then one can write \( a = m \cdot 2^p \), where \( k \) is an even integer and \( m \) is an integral multiple of \( 2u = 2^{1-r} \) such that \( 1 \leq m < 4 \). We now consider the following three cases:

- if \( m = 1 \) or \( m = 1 + 2u \), then \( \text{RN}(\sqrt{a}) = 2^{k/2} \) is an integral power of two;
- if \( m = 1 + 4u \), then \( \text{RN}(\sqrt{a}) = (1 + 2u) \cdot 2^{k/2} \) and the relative error is less than \( 2u^2 \), and thus less than \( u/\sqrt{1 + 6u} \) (since in this case we necessarily have \( p \geq 2 \));
- if \( m \geq 1 + 6u \), then, since \( \sqrt{a} \in [2^{k/2}, 2^{k/2+1}] \),
\[
\left| \text{RN}(\sqrt{a}) - \sqrt{a} \right| \leq \frac{u \cdot 2^{k/2}}{\sqrt{a}} = \frac{u}{\sqrt{m}} \leq \frac{u}{\sqrt{1 + 6u}}.
\]

If we compare with (6), we see that the above lemma gives a slightly smaller bound, since
\[
\frac{u}{\sqrt{1 + 6u}} = u - 3u^2 + O(u^3),
\]
whereas
\[
1 - \frac{1}{\sqrt{1 + 2u}} = u - \frac{3}{2} u^2 + O(u^3).
\]

Lemma III.2. Let \( a \) and \( b \) be two floating-point numbers, with \( b \) nonzero. If \( b \) is not equal to \( 2^{-2u} \) times an integral power of 2, then
\[
\text{RN} \left( \frac{a}{b} \right) = \frac{a}{b} (1 + \delta), \quad |\delta| \leq \frac{u}{1 + 3u}.
\]
Proof. Up to scaling by suitable powers of two, we can assume that \( 1 \leq b < 2 \) and \( 1 \leq a/b < 2 \), so the assumption on \( b \) becomes \( b \leq 2 - 4u \). If \( a = b \) then the division is exact, so it remains to consider the case where \( a > b \), that is, \( a/b > b + 2u \). Consequently,
\[
\frac{a}{b} - 1 \geq \frac{2u}{b} \geq \frac{1}{1 - 2u} > 1 + u,
\]
and three cases can occur:

- if \( a/b \leq 1 + 2u \), then \( \text{RN}(a/b) = 1 + 2u \) and the relative error satisfies
\[
\left| \text{RN}(a/b) - a/b \right| \leq \frac{1 + 2u}{1 + \frac{u}{1/2a}} - 1 = \frac{u(1 - 4u)}{1 - u},
\]
with the latter quantity being less than \( u/(1 + 3u) \) for \( u > 0 \);
- if \( 1 + 2u < a/b < 1 + 3u \), then \( \text{RN}(a/b) = 1 + 2u \) and
\[
\left| \text{RN}(a/b) - a/b \right| < 1 - \frac{1 + 2u}{1 + 3u} = \frac{u}{1 + 3u};
\]
- if \( a/b \geq 1 + 3u \), then, using the fact that \( a/b < 2 \),
\[
\left| \text{RN}(a/b) - a/b \right| \leq \frac{u}{a/b} \leq \frac{u}{1 + 3u};
\]

Note that \( u/(1 + 3u) = u - 3u^2 + O(u^3) \), which is slightly smaller than the expression \( u - 2u^2 \) in (7).

We can now exploit these two lemmas as follows, by considering three different cases depending on the shape of the floating-point number
\[
\hat{x} = \text{RN}(\sqrt{u/2})
\]
produced at step 6 of Algorithm 1:

1) If \( \hat{x} \) is an integral power of 2, then the floating-point division at step 7 is exact. Hence \( y = b/(2\hat{x}) \) and it follows from (10) that
\[
\hat{y} \leq y \cdot \frac{1}{L'},
\]
where \( 1/L' \) has the form
\[
1 + \frac{5}{2} u + O(u^2)
\]
and is less than \( 1 + \frac{7}{2} u \) for \( u \leq 1/2 \).

2) If \( \hat{x} = (2 - 2u) \cdot 2^k \) for some integer \( k \), then \( \sqrt{u/2} \geq (2 - 3u) \cdot 2^k \) and the relative error due to rounding is at most \( u/(2 - 3u) = u/2 + O(u^2) \). This means that instead of \( L' \) as in (9), one can take
\[
L' := \left( 1 - \frac{u}{1+u} \right) \cdot \frac{1}{(1+2u)^{1/4}} \cdot \left( 1 - \frac{u}{2 - 3u} \right)
\]
\[
= 1 - 2u + O(u^2)
\]
and replace the upper bound in (11) by
\[ \hat{y} \leq y \cdot \frac{1 + u - 2u^2}{L''}. \]
Here \((1 + u - 2u^2)/L''\) has the form
\[ 1 + 3u + \frac{15}{8}u^2 + O(u^3) \]
and is less than \(1 + \frac{7}{8}u\) for \(u \leq 1/8\).

3) In all the other cases, Lemmas III.1 and III.2 imply that
\[ \hat{x} = \sqrt{\frac{\nu}{2}} \cdot (1 + \delta), \quad |\delta| \leq \frac{u}{1 + 6u} \]
and
\[ \hat{y} = \frac{b}{2x} \cdot (1 + \delta'), \quad |\delta'| \leq \frac{u}{1 + 3u}. \]
Therefore, the upper bound in (11) can be replaced by
\[ \hat{y} \leq y \cdot \frac{1 + u + 3u}{L''}, \]
where
\[ L'' := \left( 1 - \frac{u}{1 + u} \right) \cdot \left( 1 + 3u + \frac{15}{8}u^2 + O(u^3) \right). \]
It can then be checked that \((1 + u/(1 + 3u))/L''\) has the form
\[ 1 + \frac{7}{2}u - \frac{7}{8}u^2 + O(u^3) \]
and is less than \(1 + \frac{7}{8}u\) for \(u \leq 1/8\).

The three cases above thus show that \(\hat{y} \leq y (1 + \frac{7}{8}u)\)
if \(p \geq 3\). By combining this upper bound with the lower bound in (12), we conclude that
\[ |\hat{y} - y| \leq \frac{7}{2}u|y| \quad \text{if } p \geq 3. \]

IV. CONCLUSION

The refined bounds \(\hat{x} u\) and \(\hat{z} u\) we have obtained on the relative errors of \(\hat{x}\) and \(\hat{y}\) can also be used to deduce the refined bound \(\sqrt{37} u\) on the normwise relative error \(\|z - \hat{z}\|/\|z\|\).

To see this, one can proceed exactly as Hull, Fairgrieve, and Tang in [2, p. 230]. The normwise error satisfies
\[ \frac{|\hat{z} - z|}{\|z\|} = \frac{\sqrt{(x - x)^2 + (y - y)^2}}{\sqrt{x^2 + y^2}} \]
\[ \leq \frac{\sqrt{\frac{25}{4}u^2x^2 + \frac{49}{4}u^2y^2}}{\sqrt{x^2 + y^2}} =: f(x, y) \quad \text{for } p \geq 3. \]
Since \((a, b) \neq (0, 0)\) and \(a \geq 0\) by assumption, we have \(x > 0\) and \(0 \leq y \leq x\). On this domain, \(f(x, y)\) is largest when \(x = y\, and its maximum equals
\[ f(x, x) = \frac{\sqrt{\frac{25}{4} + \frac{49}{4}}}{\sqrt{2}} u = \frac{\sqrt{37}}{2} u. \]

To summarize, we have shown the following:

**Theorem IV.1.** Assume binary floating-point arithmetic with precision \(p \geq 3\) and rounding to nearest. Then, in the absence of underflow and overflow, the floating-point values \(\hat{x}\) and \(\hat{y}\) computed by Algorithm 1 satisfy
\[ |\hat{x} - x| \leq \frac{5}{2}u|x|, \quad |\hat{y} - y| \leq \frac{7}{2}u|y|, \quad |\hat{z} - z| \leq \frac{\sqrt{37}}{2}u|z|, \]
where \(\hat{z} = \hat{x} + iy, z = x + iy, and \sqrt{37}/2 = 3.041\ldots\)

We also note that these bounds are reasonably sharp. For example,
- for \(p = 24\) (binary32/single-precision format) and with \(a = 538777/223\) and \(b = 8433897/222\), the values \(\hat{x}\) and \(\hat{y}\) computed by Algorithm 1 satisfy
\[ |\hat{x} - x|/|x| > 2.459u, |\hat{y} - y|/|y| > 3.446u, \text{ and } |\hat{z} - z|/|z| > 2.992u; \]
- for \(p = 53\) (binary64/double-precision format) and with
\[ a = 650824205667/2^{52} \]
and
\[ b = 4507997673885435/251, \]
these errors are larger than 2.482u, 3.481u, and 3.023u, respectively;
- for \(p = 113\) (binary128/quad-precision format) and with
\[ a = 596435516542135881116272475452111/2^{150} \]
and
\[ b = 5192298808565739300701174676465959/2^{111}, \]
these errors are larger than 2.483u, 3.471u, and 3.018u, respectively.

ACKNOWLEDGMENT

This research was supported in part by the French National Research Agency under grant ANR-13-INSE-0007 (MetaLibm project).

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