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

Claude-Pierre Jeannerod* and Jean-Michel Muller†

*Univ Lyon, Inria, CNRS, ENS de Lyon, Université Claude Bernard Lyon 1, LIP UMR 5668, F-69007 LYON, France,
†Univ Lyon, CNRS, ENS de Lyon, Inria, Université Claude Bernard Lyon 1, LIP UMR 5668, F-69007 LYON, France

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 $+, -, \times, \div, \sqrt{}$ 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 $7u$ and $\frac{2\sqrt{2}u}{p}$, 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

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

(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

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

and

$$y = \pm \sqrt{\frac{h - a}{2}}.$$

(2)

(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 sign$(y) = \text{sign}(b)$ with 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 $b^2 \ll a^2$, 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

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

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: $\tilde{x} \leftarrow \text{RN}(\sqrt{\nu/2})$
7: $\tilde{y} \leftarrow \text{RN}(b/(2\tilde{x}))$

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 $t$,
\[
\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq u := 2^{-p},
\]
(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 $\frac{1}{2} u + O(u^2)$, 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]:
\[
\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq \frac{u}{1 + u}.
\]
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 $b$ two floating-point numbers. If $a \geq 0$, then
\[
\text{RN}(\sqrt{a}) = \sqrt{a}(1 + \delta), \quad |\delta| \leq 1 - \frac{1}{\sqrt{1 + 2u}};
\]
if $b \neq 0$, then
\[
\text{RN}\left(\frac{a}{b}\right) = \frac{a}{b}(1 + \delta), \quad |\delta| \leq u - 2u^2.
\]
Recalling that $x = \sqrt{(h+a)/2}$, it follows that $\sqrt{\nu/2}$ satisfies
\[
x \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{(1+2u)^{3/4}} \leq \nu
\]
\[
\leq x \left(1 + \frac{u}{1 + u}\right) \left(2 - \frac{1}{\sqrt{1 + 2u}}\right)^{1/2}.
\]
By applying (6) once again, we find that the value $\hat{x}$ 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 $U' \leq 1 + \frac{5}{2} u$, 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 \(\hat{y} = \text{RN}(b/(2\hat{x}))\) produced by the last step of Algorithm 1.

Recalling that \(y = b/(2x)\), we deduce from the bounds on \(x\) in (8) that
\[
\frac{y}{U'} \leq \frac{b}{2x} \leq \frac{y}{L'}.
\]
(10)

Applying (7) then shows that \(\hat{y}\) satisfies
\[
y \cdot \left(1 - \frac{1}{2}u + 2u^2\right) \leq \hat{y} \leq y \cdot \left(1 + \frac{1}{2}u - 2u^2\right).
\]
(11)

One has
\[
\frac{1 - u + 2u^2}{U'} = 1 - \frac{7}{2}u + \frac{97}{8}u^2 + O(u^3)
\]
and one can check that this is larger than \(1 - \frac{7}{2}u\). However, the upper bound has the form
\[
\frac{1 + u - 2u^2}{L'} = 1 + \frac{7}{2}u + \frac{13}{8}u^2 + O(u^3)
\]
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 \(a = m \cdot 2^k\), where \(k\) is an even integer and \(m\) is an integral multiple of \(2u = 2^k/p\) such that \(1 \leq m < 4\). We now consider the following three cases:

- if \(m = 1\) or \(m = 1 + 2\), then \(\text{RN}(\sqrt{a}) = 2^{k/2}\) is an integral power of two;
- if \(m = 1 + 4\), 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 \(m \geq 1 + 6\), then, since \(\sqrt{a} \in [2^{k/2}, 2^{k/2+1})\),
\[
\frac{\text{RN}(\sqrt{a}) - \sqrt{a}}{\sqrt{a}} \leq \frac{u \cdot 2^{k/2}}{\sqrt{a}} = \frac{u}{\sqrt{m}} \leq \frac{u}{\sqrt{1 + 6u}}.
\]

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, \(a/b > 1 + 2u\). Consequently,
\[
\frac{a}{b} > 1 + 2u > 1 + u - 2u > 1 + u,
\]
and three cases can occur:

- if \(a/b \leq 1 + 2u\), then \(\text{RN}(a/b) = 1 + 2u\) and the relative error satisfies
\[
\left|\frac{\text{RN}(a/b) - a/b}{a/b}\right| = \frac{1 + 2u}{1 + (2u)^2} - 1 = \frac{u(1 - 4u)}{1 - u},
\]
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
\[
\left|\frac{\text{RN}(a/b) - a/b}{a/b}\right| < 1 - \frac{1 + 2u}{1 + 3u} = \frac{u}{1 + 3u};
\]
- if \(a/b \geq 1 + 3u\), then, using the fact that \(a/b < 2\),
\[
\left|\frac{\text{RN}(a/b) - a/b}{a/b}\right| \leq \frac{u}{|a/b|} \leq \frac{u}{1 + 3u}.
\]

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 \(\hat{x} = \text{RN}(\sqrt{\nu/2})\) 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 \(\hat{y} = b/(2\hat{x})\) 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 \(\sqrt{\nu/2} \geq (2 - 3u) \cdot 2^k\) 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
\[
L'' := \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{1 + (2u)^2/3} \cdot \left(1 - \frac{u/2}{2 - 3u}\right)
= 1 - 2u + O(u^2)
\]
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
\[ \hat{x} = \sqrt{\frac{\nu}{2}} \cdot (1 + \delta), \quad |\delta| \leq \frac{u}{\sqrt{1 + 6u}} \]
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
\[ L'' := \left(1 - \frac{u}{1 + u}\right) \cdot \frac{1}{(1 + 2u)^{1/4}} \cdot \left(1 - \frac{u}{\sqrt{1 + 6u}}\right). \]

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 \(\hat{y}u\) we have obtained on the relative errors of \(\hat{x}\) and \(\hat{y}\) can also be used to deduce the refined bound \(\sqrt{\frac{\nu}{2}}u\) on the normwise relative error \(|\hat{z} - z|/|z|\).

To see this, one can proceed exactly as Hull, Fairgrieve, and Tang in [2, p. 230]. The normwise error satisfies
\[ |\hat{z} - z| \leq \frac{\sqrt{(\hat{x} - x)^2 + (\hat{y} - y)^2}}{x^2 + y^2} \]
\[ \leq \frac{\sqrt{25}}{4}u^2x^2 + \frac{49}{4}u^2y^2}{x^2 + y^2} = f(x, y) \quad \text{for } p \geq 3. \]

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
\[ f(x, x) = \frac{\frac{25}{4} + \frac{49}{4}}{\sqrt{2}}u = \frac{\sqrt{37}}{2}u. \]

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 \(\hat{z} = \hat{x} + i\hat{y}, \ z = x + iy, \) 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 \(a = 53877/2^{23}\) and \(b = 843897/2^{22}\), the values \(\hat{x}\) and \(\hat{y}\) computed by Algorithm 1 satisfy \(|\hat{x} - x|/|x| > 2.459u, |\hat{y} - y|/|y| > 3.446u, \) and \(|\hat{z} - z|/|z| > 2.992u; \)
- for \(p = 53\) (binary64/double-precision format) and with \(a = 650824205667/2^{52}\)
and \(b = 450799763885435/2^{51}\), these errors are larger than \(2.482u, 3.481u, \) and \(3.023u, \) respectively;
- for \(p = 113\) (binary128/quad-precision format) and with \(a = 596435516542135881162724754522111/2^{150}\)
and \(b = 5192298808565739300701174676465595/2^{111}\),
these errors are larger than \(2.483u, 3.471u, \) and \(3.018u, \) respectively.

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**References**