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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  $+$ ,  $-$ ,  $\times$ ,  $\div$ ,  $\sqrt{\phantom{x}}$  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  $\frac{7}{2}u$  and  $\frac{\sqrt{37}}{2}u$ , 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

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

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  $b^2 \ll a^2$ , 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

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

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

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

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

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  $t$ ,

$$\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq u := 2^{-p}, \quad (4)$$

they show that the computed floating-point numbers  $\hat{x}$  and  $\hat{y}$  satisfy

$$\frac{|\hat{x} - x|}{|x|} \leq \frac{5}{2}u + \mathcal{O}(u^2)$$

and

$$\frac{|\hat{y} - y|}{|y|} \leq \frac{7}{2}u + \mathcal{O}(u^2);$$

they also show that for  $\hat{z} = \hat{x} + i\hat{y}$  and  $z = x + iy$ , the associated normwise relative error  $|\hat{z} - z|/|z|$  admits a bound smaller than  $\frac{7}{2}u + \mathcal{O}(u^2)$ , namely,

$$\frac{|\hat{z} - z|}{|z|} \leq \frac{\sqrt{37}}{2}u + \mathcal{O}(u^2), \quad \frac{\sqrt{37}}{2} = 3.041\dots$$

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  $\mathcal{O}(u^2)$  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]:

$$\text{RN}(t) = t(1 + \delta), \quad |\delta| \leq \frac{u}{1+u}. \quad (5)$$

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

$$\text{RN}(\sqrt{a}) = \sqrt{a}(1 + \delta), \quad |\delta| \leq 1 - \frac{1}{\sqrt{1+2u}}; \quad (6)$$

if  $b \neq 0$ , then

$$\text{RN}\left(\frac{a}{b}\right) = \frac{a}{b}(1 + \delta), \quad |\delta| \leq u - 2u^2. \quad (7)$$

As we shall see in §II, 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 §III. We conclude in §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

$$a^2 \left(1 - \frac{u}{1+u}\right) \leq s_a \leq a^2 \left(1 + \frac{u}{1+u}\right)$$

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

$$\begin{aligned} L &:= \left(1 - \frac{u}{1+u}\right) \cdot \frac{1}{\sqrt{1+2u}} \\ &= 1 - 2u + \frac{7}{2}u^2 + \mathcal{O}(u^3) \end{aligned}$$

and

$$\begin{aligned} U &:= \left(1 + \frac{u}{1+u}\right) \left(2 - \frac{1}{\sqrt{1+2u}}\right) \\ &= 1 + 2u - \frac{3}{2}u^2 + \mathcal{O}(u^3). \end{aligned}$$

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

$$\begin{aligned} (h+a) \left(1 - \frac{u}{1+u}\right)^2 \cdot \frac{1}{\sqrt{1+2u}} \\ \leq \nu \\ \leq (h+a) \left(1 + \frac{u}{1+u}\right)^2 \left(2 - \frac{1}{\sqrt{1+2u}}\right). \end{aligned}$$

Recalling that  $x = \sqrt{(h+a)/2}$ , it follows that  $\sqrt{\nu/2}$  satisfies

$$\begin{aligned} x \left(1 - \frac{u}{1+u}\right) \cdot \frac{1}{(1+2u)^{1/4}} \\ \leq \sqrt{\nu/2} \\ \leq x \left(1 + \frac{u}{1+u}\right) \left(2 - \frac{1}{\sqrt{1+2u}}\right)^{1/2}. \end{aligned}$$

By applying (6) once again, we find that the value  $\hat{x} = \text{RN}(\sqrt{\nu/2})$  produced at step 6 satisfies

$$xL' \leq \hat{x} \leq xU', \quad (8)$$

where

$$\begin{aligned} L' &:= \left(1 - \frac{u}{1+u}\right) \cdot \frac{1}{(1+2u)^{3/4}} \\ &= 1 - \frac{5}{2}u + \frac{41}{8}u^2 + \mathcal{O}(u^3) \end{aligned} \quad (9)$$

and

$$\begin{aligned} U' &:= \left(1 + \frac{u}{1+u}\right) \left(2 - \frac{1}{\sqrt{1+2u}}\right)^{3/2} \\ &= 1 + \frac{5}{2}u - \frac{11}{8}u^2 + \mathcal{O}(u^3). \end{aligned}$$

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  $\hat{x}$  in (8) that

$$\frac{y}{U'} \leq \frac{b}{2\hat{x}} \leq \frac{y}{L'}. \quad (10)$$

Applying (7) then shows that  $\hat{y}$  satisfies

$$y \cdot \frac{1 - u + 2u^2}{U'} \leq \hat{y} \leq y \cdot \frac{1 + u - 2u^2}{L'}. \quad (11)$$

One has

$$\frac{1 - u + 2u^2}{U'} = 1 - \frac{7}{2}u + \frac{97}{8}u^2 + \mathcal{O}(u^3)$$

and one can check that this is larger than  $1 - \frac{7}{2}u$ . However, the upper bound has the form

$$\frac{1 + u - 2u^2}{L'} = 1 + \frac{7}{2}u + \frac{13}{8}u^2 + \mathcal{O}(u^3)$$

and is *not* smaller than  $1 + \frac{7}{2}u$ . Thus, at this stage, all we have is

$$y \left(1 - \frac{7}{2}u\right) \leq \hat{y} \leq y \left(1 + \frac{7}{2}u + \mathcal{O}(u^2)\right). \quad (12)$$

To remove the term  $\mathcal{O}(u^2)$ , 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  $2u = 2^{1-p}$  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  $\sqrt{a} \in [2^{k/2}, 2^{k/2+1})$ ,

$$\frac{|\text{RN}(\sqrt{a}) - \sqrt{a}|}{\sqrt{a}} \leq \frac{u \cdot 2^{k/2}}{\sqrt{a}} = \frac{u}{\sqrt{m}} \leq \frac{u}{\sqrt{1+6u}}.$$

□

If we compare with (6), we see that the above lemma gives a slightly smaller bound, since

$$\frac{u}{\sqrt{1+6u}} = u - 3u^2 + \mathcal{O}(u^3),$$

whereas

$$1 - \frac{1}{\sqrt{1+2u}} = u - \frac{3}{2}u^2 + \mathcal{O}(u^3).$$

**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,  $a \geq b + 2u$ . Consequently,

$$\frac{a}{b} \geq 1 + \frac{2u}{b} \geq 1 + \frac{u}{1-2u} > 1 + u,$$

and three cases can occur:

- if  $a/b \leq 1 + 2u$ , then  $\text{RN}(a/b) = 1 + 2u$  and the relative error satisfies

$$\left| \frac{\text{RN}(a/b) - a/b}{a/b} \right| \leq \frac{1 + 2u}{1 + \frac{u}{1-2u}} - 1 = \frac{u(1-4u)}{1-u},$$

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  $u/(1+3u) = u - 3u^2 + \mathcal{O}(u^3)$ , 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

$$1 + \frac{5}{2}u + \mathcal{O}(u^2)$$

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  $u/(2 - 3u) = u/2 + \mathcal{O}(u^2)$ . This means that instead of  $L'$  as in (9), one can take

$$\begin{aligned} L'' &:= \left(1 - \frac{u}{1+u}\right) \cdot \frac{1}{(1+2u)^{1/4}} \cdot \left(1 - \frac{u}{2-3u}\right) \\ &= 1 - 2u + \mathcal{O}(u^2) \end{aligned}$$

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

$$1 + 3u + \frac{15}{8}u^2 + \mathcal{O}(u^3)$$

and is less than  $1 + \frac{7}{2}u$  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

$$\hat{y} = \frac{b}{2\hat{x}} \cdot (1 + \delta'), \quad |\delta'| \leq \frac{u}{1 + 3u}.$$

Therefore, the upper bound in (11) can be replaced by

$$\hat{y} \leq y \cdot \frac{1 + \frac{u}{1+3u}}{L'''},$$

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

$$1 + \frac{7}{2}u - \frac{7}{8}u^2 + \mathcal{O}(u^3)$$

and is less than  $1 + \frac{7}{2}u$  for  $u \leq 1/8$ .

The three cases above thus show that  $\hat{y} \leq y(1 + \frac{7}{2}u)$  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  $\frac{5}{2}u$  and  $\frac{7}{2}u$  we have obtained on the relative errors of  $\hat{x}$  and  $\hat{y}$  can also be used to deduce the refined bound  $\frac{\sqrt{37}}{2}u$  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

$$\begin{aligned} \frac{|\hat{z} - z|}{|z|} &= \frac{\sqrt{(\hat{x} - x)^2 + (\hat{y} - y)^2}}{\sqrt{x^2 + y^2}} \\ &\leq \frac{\sqrt{\frac{25}{4}u^2x^2 + \frac{49}{4}u^2y^2}}{\sqrt{x^2 + y^2}} =: f(x, y) \quad \text{for } p \geq 3. \end{aligned}$$

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  $\hat{z} = \hat{x} + i\hat{y}$ ,  $z = x + iy$ , and  $\sqrt{37}/2 = 3.041\dots$

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  $b = 8433897/2^{22}$ , 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

$$b = 4507997673885435/2^{51},$$

these errors are larger than  $2.482u$ ,  $3.481u$ , and  $3.023u$ , respectively;

- for  $p = 113$  (binary128/quad-precision format) and with

$$a = 5964355165421358811162724754522111/2^{150}$$

and

$$b = 5192298808565739300701174676465595/2^{111},$$

these errors are larger than  $2.483u$ ,  $3.471u$ , and  $3.018u$ , respectively.

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