A nearly correctly-rounded cube root

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This document describes the error analysis of the real cube root function `Cbrt` implemented in `numerics/cbrt.cpp`.

On a family of root-finding methods

We start with a historical overview of a family of root-finding methods.

In [Fan91a], Lagny first presents the iterates

$$a \mapsto \tfrac{1}{2}a + \sqrt{\tfrac{1}{4}a^2 + \frac{b}{3a}}, \tag{1}$$

hereafter the *irrational method*, and

$$a \mapsto a + \frac{ab}{3a^3 + b}, \tag{2}$$

the *rational method*, for the computation of the cube root $\sqrt[3]{a^3 + b}$, mentioning the existence of similar methods for arbitrarily higher powers. In [Fan91b] the above methods are again given, with an outline of the general method for higher powers, and a mention of their applicability to finding roots of polynomials other than $z^p - r$.

That general method is given in detail in [Fan92, p. 19]. Modernizing the notation, the general rule is as follows for finding a root of the monic polynomial of degree $p \geq 2$

$$f(z) \coloneqq z^p + c_1 z^{p-1} + \cdots + c_{p-1} z + c_p \eqqcolon z^p - R(z)$$

with an initial approximation a.

Separate the binomial expansion of $\left(x + \frac{1}{2}a\right)^p$ into alternating sums of degree p and $p - 1$ in z,

$$S_1 \coloneqq \sum_{\substack{k=0\\2|k}}^{p} \binom{p}{k} x^{p-k} \left(\tfrac{1}{2}a\right)^k \text{ and } S_2 \coloneqq \sum_{\substack{k=0\\2\nmid k}}^{p} \binom{p}{k} x^{p-k} \left(\tfrac{1}{2}a\right)^k,$$

and consider the polynomials in x

$$E_p \coloneqq S_1 - \tfrac{1}{2}R\left(x + \tfrac{1}{2}a\right) \text{ and } E_{p-1} \coloneqq S_2 - \tfrac{1}{2}R\left(x + \tfrac{1}{2}a\right).$$

Let E_{n-1} be the remainder of the polynomial division[1] of E_{n+1} by E_n.

[1] While the rest of the method is a straightforward translation, this step bears some explanations; its description in [Fan92] is

> De ces deux égalitez, ou prifes féparément, ou comparées enfemble felon la methode des problêmes plus que déterminez tirez en une valeur d'x rationelle, ou fimplement d'un degré commode.

It is assumed that the reader is familiar with this "comparison according to the method of more-than-determined problems". While the application of the root-finding method is described in painstaking detail in [Fan33], which outlines the treatment of overdetermined problems, it is perhaps this remark from [Fan97, p. 494] which lays it out most clearly:

> Il n'y a rien de nouveau à remarquer fur les Problemes plus que déterminez du quatriéme degré. La Regle générale eft d'égaler tout à zero, & de divifer la plus haute équation par la moins élevée, ou l'également élevée l'une par l'autre, continuellement jufques à ce que l'on trouve le refte ou le divifeur le plus fimple.

The iterate is $a \mapsto x + \frac{1}{2}a$, where x is a root of E_2 for the irrational method, and the root of E_1 for the rational method.

Modern calculus allows us to give a more straightfoward expression for the rational method than was available to Lagny; the proof of the following equivalence will be given at the end of this section.

Proposition. *The iterate of Lagny's rational method for a polynomial f of degree p is*

$$a \mapsto a + (p-1)\frac{(1/f)^{(p-2)}(a)}{(1/f)^{(p-1)}(a)}. \tag{3}$$

□

Names

The iterate (3) is a special case of the *Algorithmen* (A_ω^λ) defined by Schröder for an arbitrary polynomial f in [Sch70], equation (69) and p. 350; specifically, it is (A_{p-1}^0). As seen in the proof of the proposition, it is also a special case of Householder's equation (14) from [Hou70, p. 169], which generalizes it by substituting $\frac{f}{g}$ for f, and letting f be an arbitrary analytic function. The case $g \equiv 1$ is mentioned in theorem 4.4.2, and that expression is given explicitly in [SG01].

For $p = 2$ and f an arbitrary polynomial, (3) is Newton's method, presented by Wallis in [Wal85, p. 338].

For $p = 3$ and f an arbitrary polynomial, it is Halley's rational method, given in [Hal94, pp. 142–143] in an effort to generalize[2] Lagny's (2). It is usually simply known as Halley's method, as the irrational method—which likewise generalizes Lagny's irrational method for $p = 3$ while retaining constant order as the degree changes—has comparatively fallen into obscurity; see [ST95].

Considering, as remarked by [Sch70, p. 334], that a method can often be generalized from arbitrary polynomials or rational functions to arbitrary analytic functions, we call the iterate (3)

- Newton's method when $p = 2$, for arbitrary f;
- Lagny's rational method when $p > 2$ and f is a polynomial of degree p;
- Halley's (rational) method when $p = 3$ and f is not a polynomial of degree 3;
- the Lagny–Schröder method of order p otherwise.

We do not simply call this last case "Schröder's method", as it is only a special case of the methods defined in [Sch70], so that the expression would be ambiguous.

Note that we avoid the name "Householder's method" which appears in [SG01] and ulterior works, as it is variably used to refer to either (3) or to a method from a different family, namely φ_{p+1} from [Hou70, p. 168], equation (7), taking $\gamma_{p+1} \equiv 0$ in the resulting iteration; φ_3 is the iteration given in section 3.0.3 of [SG01]. As mentioned by Householder, both of those were described by Schröder a century prior anyway: Householder's (7) is Schröder's (18) from [Sch70, p. 327].

[2] Lagny's method is general, in that an iterate is given for any polynomial, albeit one whose order changes with the degree. However, while he refers to its results—and even corrects a misprint therein—, Halley did not have access to a copy of [Fan92],

> Has Regulas, cum nondum librum videram, ab amico communicatas habui

and it appears that said friend communicated only the formulæ for the cube and fifth root, as opposed to the general method and its proof, as Halley writes

> […] *D. de Lagney* […] qui cum totus fere ſit in eliciendis Poteſtatum purarum radicibus, præfertim Cubicâ, pauca tantum eaque perplexa nec ſatis demonſtrata de affectarum radicum extractione ſubjungit.

or, about Lagny's irrational method for the fifth root,

> Author autem nullibi inveniendi methodum ejuſve demonſtrationem concedit, etiamſi maxime deſiderari videatur […].

Being unaware of this generality, Halley sets out to generalize (1) and (2) to arbitrary polynomials, and does so by keeping the order constant.

Bibliographic note

Proof of the proposition

We now prove the above proposition, which, substituting the definition of Lagny's rational method, is that

$$x + \tfrac{1}{2}a = a + (p-1)\frac{(1/f)^{(p-2)}(a)}{(1/f)^{(p-1)}(a)} =: \psi(a)$$

if x is the root of E_1.

Proof. Let $E_p = d_0x^p + \cdots + d_p$, $E_{p-1} = e_0x^{p-1} + \cdots + e_{p-1}$. As shown in [Hou70, pp. 52–54], the polynomial remainders E_k are given up to a constant factor by [Hou70, p. 19] equation (23), *i.e.*, for some α,

$$\frac{E_k}{\alpha_k} = \det\begin{pmatrix}(E_p)_{p-1-k} \\ (E_{p-1})_{p-k}\end{pmatrix},$$

where the expression on the right-hand side is the *bigradient* defined in [Hou68] (3.2) or [Hou70, p. 19] (20),

$$\frac{E_k}{\alpha_k} = \det\begin{pmatrix}
d_0 & d_1 & d_2 & & \cdots & & d_{2(p-k)-3} & x^{p-k-2}E_p \\
0 & d_0 & d_1 & & \cdots & & d_{2(p-k)-4} & x^{p-k-3}E_p \\
\vdots & & \ddots & & & & \vdots & \\
0 & \cdots & 0 & d_0 & d_1 & \cdots & d_{p-k-1} & x^0E_p \\
0 & \cdots & 0 & 0 & e_0 & \cdots & e_{p-k-2} & x^0E_{p-1} \\
\vdots & & & \iddots & & & & \vdots \\
0 & 0 & e_0 & & \cdots & & e_{2(p-k)-4} & x^{p-k-2}E_p \\
0 & e_0 & e_1 & & \cdots & & e_{2(p-k)-4} & x^{p-k-2}E_p \\
e_0 & e_1 & e_2 & & \cdots & & e_{2(p-k)-3} & x^{p-k-1}E_p
\end{pmatrix} =: \det \boldsymbol{E}_k,$$

where $d_n := 0$ for $n > p$, and $e_n := 0$ for $n > p-1$.

In particular, for $k = 1$, the matrix $\boldsymbol{E}_1$ is

$$\begin{pmatrix}
d_0 & d_1 & d_2 & \cdots & d_{p-3} & d_{p-2} & d_{p-1} & d_p & 0 & \cdots & 0 & x^{p-3}E_p \\
0 & d_0 & d_1 & \cdots & d_{p-4} & d_{p-3} & d_{p-2} & d_{p-1} & d_p & \ddots & 0 & x^{p-4}E_p \\
\vdots & & \ddots & & & & & & & & & \vdots \\
0 & \cdots & 0 & d_0 & d_1 & d_2 & & \cdots & & & d_{p-2} & x^0E_p \\
0 & \cdots & 0 & 0 & e_0 & e_1 & & \cdots & & & e_{p-3} & x^0E_{p-1} \\
\vdots & & & \iddots & & & & & & & & \vdots \\
0 & 0 & e_0 & \cdots & e_{p-5} & e_{p-4} & e_{p-3} & e_{p-2} & e_{p-1} & \iddots & 0 & x^{p-5}E_{p-1} \\
0 & e_0 & e_1 & \cdots & e_{p-4} & e_{p-3} & e_{p-2} & e_{p-1} & 0 & \cdots & 0 & x^{p-4}E_{p-1} \\
e_0 & e_1 & e_2 & \cdots & e_{p-3} & e_{p-2} & e_{p-1} & 0 & 0 & \cdots & 0 & x^{p-3}E_{p-1}
\end{pmatrix}.$$

Observe that, since the value of x used in the rational method is the root of E_1, for that value of x, $\det \boldsymbol{E}_1 = 0$, *i.e.*, $\boldsymbol{E}_1$ is singular.

Lemma (Left as an exercise to the reviewer). *The matrix* $\boldsymbol{E}_1$ *is singular if and only if* $\boldsymbol{C}\left(x + \tfrac{1}{2}a\right)$ *is singular, where*

$$\boldsymbol{C}(\Psi) := \begin{pmatrix}
\Psi - a & c_0 & & & \\
-1 & c_1 & c_0 & & \\
0 & c_2 & & \ddots & \\
\vdots & \vdots & \ddots & & c_0 \\
0 & c_{p-1} & \cdots & c_2 & c_1
\end{pmatrix}$$

and $c_0 := 1$.

Proof. Observe that:

- since $\det \boldsymbol{E}_1$ is a polynomial of degree 1, all terms divisible by x^2 must cancel out in the Laplace expansion of that determinant on the last column, the determinant is equal to

$$\pm\delta_1 x E_p \mp \delta_2 E_p \pm \delta_3 E_{p-1} \mp \delta_4 x E_{p-1},$$

  where the δ_i are determinants of real matrices;

- by the same reasoning, only the linear and constant terms of the polynomials remain in the above expression, which simplifies to

$$\pm\delta_1 d_p x \mp \delta_2(d_{p-1}x + d_p) \pm \delta_3(e_{p-2}x + e_{p-1}) \mp \delta_4 e_{p-1}x;$$

- $E_1 - E_2 = S_1 - S_2$, which, by Lagny's *theoreme fondamental* [Fan92, p. 17], is $\left(x - \frac{1}{2}a\right)^p$.

The proof is a calculation. □

The proposition follows from the lemma and theorem 4.4.2 from [Hou70, p. 169]: $\psi(a)$ is Householder's (14) with $g \equiv 1$; for that value of g, theorem 4.4.2 states that (14) is the solution of (12) from the same page, which is $\det \boldsymbol{C}(\psi(a)) = 0$. By the lemma, for the value of x in Lagny's rational method, $x + \frac{1}{2}a$ solves that equation. □

Computing a real cube root

We now turn to the computation in `numerics/cbrt.cpp`.

Overview

The general approach to compute the cube root of $y > 0$ is the same as the one described in [KB01]:

1. integer arithmetic is used to get a an initial quick approximation q of $\sqrt[3]{y}$;
2. a root finding method is used to improve that that to an approximation ξ with a third of the precision;
3. ξ is rounded to a third of the precision, resulting in the rounded approximation x whose cube x^3 can be computed exactly;
4. a single high order iterate of a root finding method is used to get the final result.

Notation

We define the fractional part as $\operatorname{frac} a \coloneqq a - \lfloor a \rfloor \in [0, 1[$, regardless of the sign of a.

The quantities $p \in \mathbb{N}$ (precision in bits) and $bias \in \mathbb{N}$ are as defined in IEEE 754-2008.

We use capital letters fixed-point numbers involved in the computation, and $A > 0$ for the normal floating-point number $a > 0$ reinterpreted as a binary fixed-point number with t bits after the binary point[3],

$$\begin{aligned} A &\coloneqq bias + \lfloor \log_2 a \rfloor + \operatorname{frac}(2^{-\lfloor \log_2 a \rfloor} a) \\ &= bias + \lfloor \log_2 a \rfloor + 2^{-\lfloor \log_2 a \rfloor} a - 1, \end{aligned}$$

and *vice versa*,

$$a \coloneqq 2^{\lfloor A \rfloor - bias}(1 + \operatorname{frac} A).$$

[3]The implementation uses integers (obtained by multiplying the fixed-point numbers by 2^{p-1}). For consistency with [KB01] we work with fixed-point numbers here. Since we do not multiply fixed point numbers together, the expressions are unchanged.

This corresponds to [KB01]'s $B+K+F$.

For both fixed- and floating-point numbers, given $\alpha \in \mathbb{R}$, we write $[\![\alpha]\!]$ for the nearest representable number (rounding ties to even). For fixed-point numbers, we write $[\![\alpha]\!]_0$ for directed rounding towards 0 to the fixed-point precision (as in division implemented with integer division).

Except in the section on rescaling, the input y and all intervening floating-point numbers are taken to be normal; the rescaling performed to avoid overflows also avoids subnormals.

0.1 Quick approximation

The quick approximation q is computed using fixed-point arithmetic as

$$Q \coloneqq C + \left[\!\!\left[\frac{Y}{3}\right]\!\!\right]_0,$$

where the fixed-point constant C is defined as[4]

$$C \coloneqq \left[\!\!\left[\frac{2\,bias - \gamma}{3}\right]\!\!\right]$$

for some $\gamma \in \mathbb{R}$.

Let $\varepsilon \coloneqq \frac{q}{\sqrt[3]{y}} - 1$, so that $\sqrt[3]{y}(1+\varepsilon) = q$; the relative error of q as an approximation of $\sqrt[3]{y}$ is $|\varepsilon|$. Considering Y, Q, q, and ε as functions of y, we have

$$\begin{aligned} Y(8y) &= Y(y) + 3, \\ Q(8y) &= Q(y) + 1, \\ q(8y) &= 2q(y), \\ \varepsilon(8y) &= \varepsilon(y), \end{aligned}$$

so that the properties of ε need only be studied on some interval of the form $[\eta, 8\eta[$.

Pick $\eta \coloneqq 2^{\lfloor\gamma\rfloor}$, and $y \in [\eta, 8\eta[\;=\; [2^{\lfloor\gamma\rfloor}, 2^{\lfloor\gamma\rfloor+3}[$, so that $\log_2 y \in [\lfloor\gamma\rfloor, \lfloor\gamma\rfloor + 3[$. Let $k \coloneqq \lfloor \log_2 y\rfloor - \lfloor\gamma\rfloor$; note that $k \in \{0,1,2\}$. Let $f \coloneqq \operatorname{frac}(2^{-\lfloor \log_2 y\rfloor} y) \in [0,1[$. Up to at most 1.5 units in the last place from rounding,

$$\begin{aligned} Q \approx Q' &\coloneqq bias + \frac{\lfloor \log_2 y\rfloor}{3} + \frac{\operatorname{frac}(2^{-\lfloor \log_2 y\rfloor} y) - \gamma}{3}, \\ &= bias + \frac{\lfloor\gamma\rfloor + k}{3} + \frac{f-\gamma}{3}, \\ &= bias + \frac{k + f - \operatorname{frac}\gamma}{3}. \end{aligned}$$

Since $k \in [0,2]$, the numerator $k + f - \operatorname{frac}\gamma$ lies in $]-1,3[$. Further, it is negative only if $k=0$, so that

$$\lfloor Q'\rfloor = \begin{cases} bias - 1 & \text{if } k = 0 \text{ and } \operatorname{frac}\gamma > \operatorname{frac}(2^{-\lfloor\gamma\rfloor} y), \\ bias & \text{otherwise,} \end{cases} \quad \text{and}$$

$$\operatorname{frac} Q' = \begin{cases} 1 + \frac{f - \operatorname{frac}\gamma}{3} & \text{if } k = 0 \text{ and } \operatorname{frac}\gamma > f, \\ \frac{k+f-\operatorname{frac}\gamma}{3} & \text{otherwise.} \end{cases}$$

Accordingly, for the quick approximation q, we have, again up to at most 1.5 units in the last place,

$$q \approx q' = \begin{cases} 1 + \frac{f - \operatorname{frac}\gamma}{6} & \text{if } k = 0 \text{ and } \operatorname{frac}\gamma > f, \\ 1 + \frac{k+f-\operatorname{frac}\gamma}{3} & \text{otherwise,} \end{cases}$$

[4] Note that there is a typo in the corresponding expression $C \coloneqq (B - 0.1009678)/3$ in [KB01]; a factor of 2 is missing on the bias term.

With $\sqrt[3]{y} = 2^{\frac{\lfloor y \rfloor + k}{3}} \sqrt[3]{1+f}$, we can define

$$\varepsilon' \coloneqq \frac{q'}{\sqrt[3]{y}} - 1,$$

which we can express piecewise as a function of f and k. This gives us a bound on the relative error,

$$|\varepsilon| \le |\varepsilon'| + 1.5 \cdot 2^{p-1}(1 + |\varepsilon'|).$$

The values $\gamma = 0.1009678$ and $\varepsilon < 3.2\%$ from [KB01] may be recovered by choosing γ minimizing the maximum of $|\varepsilon'|$ over $y \in [\eta, 8\eta[$, or equivalently.

$$\gamma_{\text{Kahan}} \coloneqq \operatorname*{argmin}_{\gamma \in \mathbb{R}} \max_{y \in [\eta, 8\eta[} |\varepsilon'| = \operatorname*{argmin}_{\gamma \in \mathbb{R}} \max_{(f,k)} |\varepsilon'|$$

where the maximum is taken over $(f, k) \in [0, \operatorname{frac} \gamma[\times \{0\} \cup [0, 1[\times \{1, 2\}$,

$$= \operatorname*{argmin}_{\gamma \in \mathbb{R}} \max_{(f,k) \in \mathcal{E} \cup \mathcal{L}} |\varepsilon'|,$$

where $\mathcal{E} \coloneqq \{(\operatorname{frac} \gamma, 0)\} \cup \{(0, k) \mid k \in \{0, 1, 2\}\}$ is the set of the endpoints of the intervals whereon q' is piecewise affine, and $\mathcal{L} \coloneqq \left\{\left(\frac{k - \operatorname{frac} \gamma}{2}, k\right) \,\middle|\, k \in \{1, 2\}\right\}$ are the local extrema.

The values are more precisely[5]

$$\gamma_{\text{Kahan}} \approx 0.10096\,78121\,55802\,88786\,36993\,42643\,55358\,06489\,88235\,75289$$

with

$$\max_y |\varepsilon'| \approx 0.03155\,46327\,73624\,80606\,11789\,73328\,17135\,58940\,02093\,40816,$$

leading to $C_{\text{Kahan}} = {}_{16}\mathrm{2A9F\,7625\,3119\,D328} \cdot 2^{-52}$ for IEEE 754-2008 binary64. However, as we will see in the next section, this value does not optimize the final error, so it is not the one that we use.

0.2 Getting to a third of the precision

We use a single iterate of Lagny's rational method to compute ξ,

$$\xi \coloneqq \left[\!\left[q - \left[\!\left[\frac{[\![([\![[\![q^2]\!]q]\!] - y)q]\!]}{[\![2[\![[\![q^2]\!]q]\!] + y]\!]} \right]\!\right] \right]\!\right].$$

Note that the subtraction in the numerator is exact by Sterbenz's lemma. Let $\Delta \coloneqq \frac{\xi}{\sqrt[3]{y}} - 1$ and

$$\xi' = q' - \frac{({q'}^3 - y)q'}{2{q'}^3 + y}.$$

We have, up to rounding errors (TODO: bound those),

$$\Delta \approx \Delta' \coloneqq \frac{\xi'}{\sqrt[3]{y}} - 1.$$

With $q' = \sqrt[3]{y}(1 + \varepsilon')$, we can express Δ' using the transformation of the relative error error by one step of Lagny's rational method on the cube root,

$$\Delta' = \frac{2{\varepsilon'}^3 + {\varepsilon'}^4}{3 + 6\varepsilon' + 6{\varepsilon'}^2 + 2{\varepsilon'}^3}.$$

If q' is computed using $\gamma = \gamma_{\text{Kahan}}$, we get

$$\max_y |\Delta'| \approx 0.00002196,$$

$$\log_2 \max_y |\Delta'| \approx -15.47.$$

[5]These may be computed formally, but the expressions are unwieldy.

However, γ_{Kahan}, which minimizes $\max_y|\varepsilon|$, does not minimize $\max_y|\Delta'|$. This is because while Δ' is monotonic as a function of ε', it is not odd: positive errors are reduced more than negative errors are, so that the minimum is attained for a different value of γ. Specifically, we have

$$\begin{aligned}\gamma_{\mathrm{L}} &\coloneqq \operatorname*{argmin}_{\gamma\in\mathbb{R}} \max_y|\Delta'| \\ &\approx 0.09918\,74615\,29855\,99525\,66149\,20761\,31234\,34720\,23067\,92759\end{aligned}$$

with

$$\max_y|\varepsilon'| \approx 0.03103\,20521\,29929\,93577\,08166\,75859\,02139\,33719\,41389\,93269,$$

but

$$\max_y|\Delta'| \approx 0.00002\,08686\,35536\,39593\,48770\,92008\,39844\,10254\,14831\,61229.$$

The corresponding fixed-point constant is $C_{\mathrm{L}} \coloneqq {}_{16}\mathrm{2A9F\,7893\,782D\,A1CE} \cdot 2^{-52}$ for binary64.

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