A Correct Newton-Rhapson and a Better Halley

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The lowly fixed-point recursion $x_{n+1} = f(x_n)$, which is at the bottom of the iterative methods evolutionary ladder, should come before the Newton-Raphson method. Yet in calculus texts the latter takes precedence, due probably to the appeal of its plausible geometrical interpretation visualized so convincingly as sliding down tangent lines. But relying on graphs and pictures can lead to simplistic thinking.

FIXED-POINT ITERATION. Before considering the Newton-Raphson method, and its faster extensions, such as the Halley (of comet-discovery fame) method we briefly reconsider the fixed-point iteration method. The linear function $f(x) = k(x - a)a + a$ has a unique fixed-point $x = a$ at which $a = f(a)$ for any value of constant $k \neq 1$. For this function the fixed-point iterative method assumes the simple form $x_{n+1} = k(x_n - a) + a$ or $|x_{n+1} - a| = |k| \; |(x_n - a)|$, from

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which we conclude that if $|k| < 1$, then point x_n+1 is closer to point a than point x_n, and convergence of x_n to a takes place, independently of the starting point, $x_n \to a$ as $n \to \infty$, albeit linearly. If slope k is zero – if the line is horizontal – then convergence is immediate. This suggests the desirability of $f(x)$ in the general case of $x_{n+1} = f(x_n)$ to look like a horizontal line in the vicinity of the fixed-point, which is the essence of the following theorem.

THEOREM. Let a be a fixed-point of function $f(x)$, $a = f(a)$. Suppose $f(x)$ to have a bounded derivative of order $m + 1$ in an open interval containing fixed-point a. If $f'(x) = f''(x) = \dots = f^{(m)}(a) = 0$, but $f^{(m+1)}(a) \neq 0$, then the sequence x_n produced by $x_{n+1} = f(x_n)$ is such that $|a - x_{n+1}| < c|a - x_{n+1}|^m$, for some constant $c > 0$, provided that x_0 is taken close enough to a.

PROOF. We shall prove the theorem for the specific case of $m = 2$. Let $f'''(x)$ be bounded on the interval $I = (a - \delta, a + \delta)$, $\delta > 0$, and assume x to be in this interval. Taylor's expansion of $f(x)$ around point a is

$$f(x) = f(a) + (x - a)f'(a) + \frac{1}{2}(x - a)^2 f''(a) + \frac{1}{6}(x - a)\, f'''(\xi),\ a < \xi < x$$

if x is to the right of a. The assumptions $a = f(a)$, $f'(a) = 0$, and $f''(a) = 0$ reduce this equality to $f(x) - a = (1/6)(x - a)^3 f'''(\xi)$ or $|f(x) - a| \leq (M/6)|x - a|^3$, where M is an upper bound on $|f'''(x)|$ in I. For $x_1 = f(x_0)$ the inequality becomes

$$|x_1 - a| \leq c|x_0 - a|^3,\ c = \frac{M}{6}$$

and if $|x_1 - 0| < 1$, then $|x_0 - a|^3$ is much smaller than 1. For x_0 sufficiently close to a, x_1 is closer to a than x_0, and hence it is also in I, and so on. End of proof.

FROM FIXED-POINT ITERATION TO THE NEWTON-RHAPSON (NR) METHOD. To keep matters simple we assume that the function $f(x)$ is twice differentiable everywhere. Suppose number a exists such that $f(a) = 0$ but $f'(a) \neq 0$. We seek to iteratively generate ever better approximations to a. If constant $A \neq 0$, then $x = F(x)$; $F(x) = x + Af(x)$ is equivalent to $f(x) = 0$, for which we propose the fixed-point iteration $x_{n+1} = x_n + Af(x_n)$. To have quadratic convergence we require that $F'(a) = 0$ and we determine that $A = -1/f(a)$ so that $x_{n+1} = x_n - f(x_n)/f'(a)$, which we want to call the correct Newton-

Rhapson method. Since a is unknown we do the next best thing and replace it by x_n to have the classical NR method $x_{n+1} = x_n - f(x_n)/f'(x_n)$. To prove the quadratic convergence of the classical NR method, we derive it from the fixed-point iteration by taking $F(x) = x + g(x)f(x)$, $g(x) = A/f'(x)$ for constant A, and fix it from $F'(a) = 0$ as $A = -1$ independently of a.

For example, application of the classical NR method to $f(x) = x^2 - 1$ yields the recursion $x_{n+1} - 1 = (x_n - 1)^2/(2x_n)$ that quadratically converges to $a = x_\infty = 1$ for any $x_0 > 0$. Pretending to know that $f'(1) = 2$ we obtain from the correct NR method the recursion $x_{n+1} - 1 = (x_n - 1)^2/(2)$ that quadratically converges to $a = x_\infty = 1$ for any $-1 < x_0 < 3$.

Yet it may happen that even if root a of $f(x) = 0$ is unknown still $f'(a)$ is known via a differential equation for f. Consider using the NR method for computing (Epperson) the natural logarithm. Here $f(x) = e^{x} - \alpha$, the root of which is $a = \ln\alpha$, and $f'(a) = \alpha$. The classical NR method for this function is $x_{n+1} = x_n - (e^{x_n} - \alpha)/e^{x_n}$, while the *correct* NR method is here $x_{n+1} = x_n - (e^{x_n} - \alpha)/\alpha$. Practically, the two methods may not be far apart, but if $f'(a)$ is known, it would seem silly not to apply the correct NR method.

HALLEY'S AND HIGHER ORDER METHODS. We write $x = F(x)$, $F() = x + g(x)f(x)$ so that the fixed-point a of F is a root of f, $f(a) = 0F(x)$, if $g(a) \neq 0$, and we consider the fixed-point iterative method $x_{n+1} = F(x_n)$. We differentiate $F(x)$ twice to have

$$F'(x) = 1 + gf' + g'f \text{ and } F''(x) = gf'' + 2g'f' + g''f$$

and if $F'(a) = F''(a) = 0$, then the sequence generated by the recursion $x_{n+1} = F(x_n)$ is under propitious circumstances, cubically converging to fixed-point a. But we do not know a. We recall having obtained the correct NR method from the fixed-point iteration method under the assumption that weight function $g(x_n)$ is constant, or $g' = g'(x_n) = 0$. Here we assume $g''(x_n) = 0$. Not knowing fixed-point a we replace the conditions $F'(a) = 0$ and $F''(a) = 0$ by $F'(x_n) = 0$. By this, mitigating conditions g and g' are obtained from the linear system

$$\begin{bmatrix} f' & f \\ f'' & 2f' \end{bmatrix} \begin{bmatrix} g \\ g' \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \end{bmatrix} \text{ and } \quad g = \frac{\det\begin{bmatrix} -1 & f \\ 0 & 2f' \end{bmatrix}}{\det\begin{bmatrix} f' & f \\ f'' & 2f' \end{bmatrix}} = \frac{-2f'}{2f'^2 - f'f''}$$

where f, g and their derivatives are all evaluated at x_n. Now

$$x_{n+1} = x_n - \frac{2f'_n}{2f'^2_n - f_n f''_n} f_n$$

which is Halley's method (Gander).

To observe its cubic convergence we select $f(x) = x^2 - 1$, for which $f' = 2x$ and $f'' = 2$, and readily ascertain that $x_{n+1} - 1 = (1/(1 + 3x_n^2))(x_n - 1)^3$, or $x_{n+1} - 1 = (1/4)(x_n - 1)^3$ if $x_n = 1$, nearly.

To prove the cubic convergence of Halley's method we write is as $x_{n+1} = F(x_n)$ for $F(x) = x + g(x)f(x)$ and $g(x) = -2f/2f'^2 - ff'')$. We verify that $g(a) = -1/f'(a)$ and $g'(a) = f''(a)/(2f'^2(a))$ for a such that $f(a) = 0$. It follows that $F'(a) = F''(a) = 0$, and we conclude that convergence is indeed cubic for $f(x)$ satisfynig the hypothesis of the general fixed-point iteration theorem.

Emboldened by our success in procuring the quadratic Newton-Rhapson method and the cubic Halley method from the fixed-point iteration method we venture to create a hopefully *quartic* iterative method by letting $F'(x_0) = 0$, $F''(x_0) = 0$ and $F'''(x_0) = 0$. Differentiating $F(x) = x + gf$ we have

$$F' = 1 + gf' + g'f,\ F'' = gf'' + 2g'f' + g''f,\ F''' = gf''' + 3g'f'' + 3g''f' + g'''f$$

in which we put $g''' = g'''(x_n) = 0$, set $F' = F'' = F''' = 0$ and have the linear system of three equations in three unknowns

$$\begin{bmatrix} f' & f & 0 \\ f'' & 2f' & f \\ f''' & 3f'' & 3f' \end{bmatrix} \begin{bmatrix} g \\ g' \\ g'' \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}$$

for g, g' and g''. This system is solved as

$$g = \frac{\det \begin{bmatrix} -1 & f & 0 \\ 0 & 2f' & f \\ 0 & 3f'' & 3f' \end{bmatrix}}{\det \begin{bmatrix} f' & f & 0 \\ f'' & 2f' & f \\ f''' & 3f'' & 3f' \end{bmatrix}} = -\frac{6f'^2 - ff''}{6f'^3 - 6ff'f'' + f^2 f'''}$$

and our proposed hopefully quartic iterative method becomes

$$x_{n+1} = x_n - \frac{6f'^2_n - 3f_n f''_n}{6f'^3_n - 6f_n f'_n f''_n + f^2_n f'''_n} f_n$$

implicit in a formula of Householder (1970). To observe the order of convergence of this method we select the function $f(x) = x^2 - 1$ for which $f'(x) = 2x$, $f''(x) = 2$, $f'''(x) = 0$, and determine that $x_{n+1} - 1 = (1/(4x_n^3 + 4x_n))(x_n - 1)^4$, or $x_{n+1} - 1 = (1/8)(x_n - 1)^4$, nearly, if $x_n = 1$, nearly.

To prove the quartic convergence of this method we write it as $x_{n+1} = F(x_n)$ for $F(x) = x + g(x)f(x)$ and $g(x) = (-6f'^2 + 3ff f'')/(6f'^3 - 6ff'f'' + f^2 f''')$, where f is short for $f(x)$. We verify (using Mathematica©) that $g(a) = -1/f'$, $g'(a) = f''/(2f'^2)$ and $g''(a) = -f''^2/(2f'^3) + f'''/(3f'^2)$ where f', f'' and f''' are short for $f'(a)$, $f''(a)$ and $f'''(a)$. It readily results that $F'(a) = F''(a) = F'''(a) = 0$, proving that convergence is indeed quartic for $f(x)$ satisfying the hypothesis of the general fixed-point iteration theorem.

COMPUTATION OF SQUARE ROOTS. For $f(x) = x^2 - \alpha = 0$, $\alpha = \sqrt{\alpha}$ the NR method is $x_{n+1} = x_n - 1/(2x_n) f_n$, $f_n = f(x_n)$. For $\alpha = 2$ it becomes the ubiquitous recursion $x_{n+1} = x_n/2 + 1/x_n$, and $x_{n+1} - \sqrt{2} = (1/2x_n)(x_n - \sqrt{2})^2$ or $x_{n+1} - \sqrt{2} = (\sqrt{2}/4)(x_n - \sqrt{2})^2$, nearly, if x_n is close to $\sqrt{2}$, implying that convergence is quadratic, and from above. We suggest to reform the NR method, writing it as $x_{n+1} = x_n - x_n(x_n^2 - 2)^2/(2x_n^2)$ and set $x_n^2 = 2$ so as to have $x_{n+1} = (x_n/4)(6 - x_n^2)$. Division by x_n is thereby replaced by a multiplication. Some algebra leads to $x_{n+1} - \sqrt{2} = (1/4)(x_n + 2\sqrt{2})$ or $x_{n+1} - \sqrt{2} = (-3\sqrt{2}/4)(x_n - \sqrt{2})^2$, nearly, if x_n is close to $\sqrt{2}$, implying that convergence is quadratic, and from below. Yet we notice that the factor $-3\sqrt{2}/4$ is three times bigger in magnitude than the corresponding factor in the unaltered NR method.

It occurs to us now that since the two methods converge from opposite directions their average weighted at the ration of $3/4$ to $1/4$ should do better. Taking

$$x_{n+1} = \frac{3}{4}\,\frac{x_n^2 + 2}{2x_n} + \frac{1}{4}x_n(6 - x_n^2)$$

we obtain

$$x_{n+1} = -\frac{1}{16x_n}(x_n^4 - 12x_n^2 - 12)$$

or

$$x_{n+1} - \sqrt{2} = -\frac{x_n + 3\sqrt{2}}{16x_n}(x_n - \sqrt{2})^3$$

demonstrating that we have constructed in this way a cubic method. If $x_n = \sqrt{2}$, nearly, then $x_n - \sqrt{2} = -(1/4)(x_n - \sqrt{2})^3$, nearly, implying that the error of this cubic method alternates its sign.

The iterative scheme $x_{n+1} = (x_n + 2)/(x_n + 1)$ is such that $x_{n+1} - \sqrt{2} = c\ (x_n - \sqrt{2})$, with constant $c = (1 - \sqrt{2})/(1 + \sqrt{2})$. It occurs to us that this scheme is but a special case of the more general

$$x_{n+1} = \frac{a_1 + a_2 x_n}{b_1 + x_n}$$

and now we want to know if coefficients a_1, a_2, b_1 can be selected to have a successive errors relationship $x_{n+1} - \sqrt{2} = c\ (x_n - \sqrt{2})$ for this scheme with a smaller $|c|$ for faster convergence.

This rational relationship between x_n and x_{n+1} must correctly predict that $x_{n+1} = \sqrt{2}$ if $x_n = \sqrt{2}$, which requires that $a_1 = \sqrt{2}(b_1 - a_2) + 2$. Wanting to avoid irrational coefficients, we enforce the condition $b_1 = a_2$, and are left with $a_1 = 2$, so that

$$x_{n+1} = \frac{2 + b_1 x_n}{b_1 + x_n}$$

Algebra produces

$$x_{n+1} - \sqrt{2} = \frac{b_1 - \sqrt{2}}{b_1 + x_n}\ (x_n - \sqrt{2}),\ x_{n+1} - \sqrt{2} = c(x_0)(x_n - \sqrt{2}).$$

The smallest $|c| = 2$ is obtained with $b_1 = \sqrt{2}$, with which we have

$$x_{n+1} - \sqrt{2} = \frac{4 + \sqrt{2}\, x_n}{\sqrt{2} + x_n}$$

which is merely the trivial $x_n = \sqrt{2}$ in disguise. Wanting to exclude irrational coefficients in this recursive formula, we replace $\sqrt{2}$ with a good rational approximation q/p. Say $q/p = 7/5$. Then

$$x_{n+1} + 1 = \frac{10 + 7x_n}{7 + 5x_n}$$

for which $e_{n+1} = (7 - 5\sqrt{2})/(7 + 5\sqrt{2})e_n$, $e_n = x_n - \sqrt{2}$.

We may turn the static recursion $x_{n+1} = (2 + b_1 x_n)/(b_1 + x_n)$, with a constant b_1 that is a good approximation to $\sqrt{2}$, into a dynamic recursion in which b_1 is repeatedly changed as better and better approximations become available for $\sqrt{2}$. Taking $b_1 = x_0$ we obtain the NR recursion $x_{n+1} = (x_n^2 + 2)/(2x_n)$, which is quadratically convergent.

To obtain a quartic method from the general fixed-point iteration theorem we propose to write $f(x) = 0$ as $x = x + f(x)g(x)$, or, shortly, $x = F(x)$, for $g = x^{-1}(A + Bx^2 + Cx^4)$, and fix constants A,B,C so that $F'(a) = F''(a) = F'''(a) = 0$. The special choice of weight function g is designed to assure the explicit dependence of A,B,C on α but not on a. In fact,

$$A = -\frac{5}{16}\,,\ B = -\frac{1}{4\alpha},\ \text{and}\ C = \frac{B}{4\alpha} = -\frac{1}{16\alpha^2}\,.$$

Similarly, for the rational choice

$$g(x) = \frac{1}{x}\,\frac{A + Bx^2}{1 + Cx^2}$$

we compute

$$A = -\frac{1}{4}\,,\ B = -\frac{3}{4\alpha},\ \text{and}\ C = \frac{1}{\alpha}\,.$$

To numerically compare the NR method to the two quartic methods we select $\alpha = 2$ and $x_0 = 1$. We consider the iterative method convergenced as soon as x_n has reached 16 correct digits. For these values the NR method converges in five steps, but the quartic in three. Of course, the computational efficiency of the different methods must also be considered, but it is not for now.

For

$$g(x) = x^{-1}(A + Bx^2 + Cx^4 + Dx^6$$

we obtain

$$A = -\frac{35}{128},\ B = -\frac{47}{128\alpha},\ C = \frac{23}{128\alpha^2}\,,\ \text{and}\ D = -\frac{5}{128\alpha^3}$$

while for

$$g(x) = \frac{1}{x} \; \frac{A + Bx^2 + Cx^4}{1 + Dx^2 + Ex^4}$$

we get

$$A = -\frac{1}{6}, B = -\frac{5}{3\alpha}, C = -\frac{5}{6\alpha^2}, D = -\frac{10}{3\alpha}, \text{ and } D = -\frac{1}{\alpha^2}.$$

Convergence with these last two methods is in two steps.

COMPUTATION OF THE NATURAL LOGARITHM. To obtain a higher order fixed-point iteration method for the root $a = \ln\alpha$ of $f(x) = e^x - \alpha = 0$ we write it as $x = F(x)$ with $F(x) = x + g(x)f(x)$, $g(x) = A + e^x + Ce^{2x}$ and fix constants A, B, and C so that $F'(a) = F''(a) = F'''(a) = 0$. The success of this choice of $g(x)$ hinges on the fact that A, B, and C are independent of a. Repeatedly differentiating $F(x) = x + g(x)f(x)$ we have $F' = 1 + g'f + gf'$, $F'' = g''f + 2g'f' + gf''$, and $F''' = g'''f + 3g''f' + 3g'f''' + gf''$, from which we obtain by means of some simple algebra

$$A = -\frac{11}{6\alpha}, B = \frac{7}{6\alpha^2}, C = -\frac{1}{3\alpha^3}$$

and forthwith the quartic method

$$x_{n+1} = x_n + \left(-\frac{11}{6\alpha} + \frac{7}{6\alpha^2}e_n - \frac{1}{3\alpha^3}e_n^2\right)(e_n - \alpha), \; e_n = e^{x_n}$$

that requires the computation of e^x in each iterative cycle only once.

Halley's method applied to $f(x) = e^x - \alpha$ yields the recursion

$$x_{n+1} = x_n - \frac{2}{e_n - \alpha}(e_n - \alpha), \; e_n = e^{x_n}.$$

Correspondingly, we propose the rational recursion

$$x_{n+1} = x_n + \frac{A + Be_n}{1 + Ce_n}(e_n - \alpha), \; e_n = e^{x_n}$$

for which we find

$$A = -\frac{5}{2\alpha}, \ B = -\frac{1}{2\alpha^2}, \ C = \frac{2}{2\alpha}.$$

To compare the two methods numerically we choose $\alpha = 2$, so that root $a = \ln(2)$, and take as starting value $x_0 = 1$. Halley's method converged in three steps and our rational method converged in two steps. One can not ask for more than a two step convergence, as one step is needed to come close to the root, and one more to be at it.

COMPUTATION OF THE EXPONENTIAL FUNCTION. To find the root of $f(x) = \ln x - \alpha$ we propose

$$x_{n+1} = x_n + x_n(A + B\ln x_n + C\ln^2 x_n)(\ln x_n - \alpha)$$

but decide to take $C = 0$ and find $A = -1 - \alpha/2$, $B = 1/2$. Halley's method applied to this function yields the recursion

$$x_{n+1} = x_n - \frac{2x_n}{2 - \alpha + l_n}(l_n - \alpha), \ l_n = \ln x_n.$$

Correspondingly, we propose

$$x_{n+1} = x_n + x_n \frac{A + B l_n}{1 + C l_n}(l_n - \alpha), \ l_n = \ln x_n$$

and find

$$A = \frac{6 + \alpha}{-6 + 2\alpha}, \ B = \frac{1}{6 - 2\alpha}, \ C = \frac{1}{3 - \alpha}.$$

We numerically compare the two methods for $\alpha = 0.5$, $a = \sqrt{e}$, starting with $x_0 = 0$. Once more, Halley's method converges in three steps and our rational method in only two.

COMPUTATION OF ARCSIN. Once a good program is available for the evaluation of sin x and cos x, $0 < x < \pi/2$, the trigonometric function arcsin x

can be obtained as the solution of sin $x - \alpha = 0$. For a cubic iterative solution method we propose to $g(x) = A + B \cos x$, and we ascertain that $F(a) = F''(a) = 0$ if $A = (3\alpha^2 - 2)/(2\beta^3)$ and $B = -\alpha/(2\beta^3)$, where $\beta = \sqrt{1 - \alpha^2}$. To have a quartic method we suggest $g(x) = (A + B \cos x)/(1 + C \cos x)$ and ascertain that $F(a) = F''(a) = F'''(a) = 0$ if

$$A = \frac{\beta}{1 + 2\alpha^2} - \frac{2}{\beta},\ B = \frac{1}{1 + 2\alpha^2},\ C = \frac{-2\beta}{1 + 2\alpha^2} + \frac{1}{\beta},\ \text{where } \beta = \sqrt{1 - \alpha^2}.$$

Halley's method is here

$$x_{n+1} = x_n - \frac{2c_n}{c_n^2 - \alpha s_n}(s_n - \alpha) \text{ where } c_n = \cos x_n, \text{ and } s_n = \sin x_n$$

We numerically compare the two methods for $\alpha = 0.5$, $a = \arcsin(0.5) = \pi/6$, starting with $x_0 = 1$. Using high precision computation to supress the ill effect of arithmetical round-off, we observe Halley's method converges in four steps, and our rational method in only two.

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