Estimated Error Bounds from Cauchy's Iterating Function

Absent an explicit formula for the desired real root z of a given equation $f(z) = 0$, the equation is transformed into the form of a fixed-point problem: " Find $z = U(z)$ ", and then an iteration $x_{n+1} := U(x_n)$ starts from some x_0 close enough to z that $x_n \to z$ as $n \to +\infty$, we hope. A typical example is *Newton's Iterating Function*: $\ddot{U}(x) := x - f(x)/f'(x)$. Its iteration converges *Quadratically* to a simple zero z of f, but only *Linearly* to a multiple zero; in particular, when converging to a double zero z each iteration roughly halves the error $x_n - z$.

At the cost of computing the second derivative $f''(x)$ too, faster convergence is provided by

Cauchy's iterating function $\hat{U}(x) := x - 2\,(f(x)/f'(x))/\big(1 + \sqrt{(1 - 2\,f''(x)\,f(x)/f'(x)^2)}\big)$.

Its iteration converges *Cubically* to a simple zero, and to a double zero with order at least 3/2. Indeed, if f and the desired zero are both real, substituting zero for any imaginary $\sqrt{\ldots}$ that occurs during the computation of Cauchy's iterating function, thus evading complex arithmetic, can only hasten convergence towards a double zero, raising the order to quadratic. Normally, when z is a simple zero, Cauchy's cubic convergenge is computationally faster than Newton's quadratic when, as is usually the case, the computation of f'' adds less than 58% more time to the computation of f and f'. Verification of the foregoing assertions is left to diligent readers.

When f and its first two derivatives take a long time to compute, stopping the iteration as soon as possible becomes urgent. To this end a modest over-estimate of the current iterate's error will play an indispensable role in the stopping criterion. Such an over-estimate is the goal of this note.

Suppose a program intended to solve $f(z) = 0$ actually computes $\mathrm{f}(x) := f(x) - \delta\mathrm{f}$ because of roundoff's intervention. Then, instead of z, the best we can expect from the program is a zero $z + \delta z$ of $\mathrm{f}(x)$. If z is a simple zero far from every other zero and singularity of f, Newton's iteration supplies a fair estimate for δz, namely $\delta z \approx \delta\mathrm{f}/f'(z)$. But when f has two zeros z and $z - \Delta z$ close to each other but far from every other zero and singularity, so that $f''(x)$ varies relatively slowly for x near z and $z - \Delta z$, Cauchy's iterating function offers a better estimate

$$\delta z \approx 2\,(\delta\mathrm{f}/f'(z))/\big(1 + \sqrt{(1 + 2\,f''(z)\,\delta\mathrm{f}/f'(z)^2)}\big)$$

though it may become complex. Normally we cannot know f 's error $\delta\mathrm{f}$; if we knew it we'd get rid of it. Instead, our error-analyses estimate the computed f 's *Uncertainty*, which is how big $|\delta\mathrm{f}|$ cannot be;— it is a rough *Error Bound*. Combine this with an application of the inequality

$$|\,h/(1 + \sqrt{1-h})\,| \le |h|/|\,1 + \sqrt{1-|h|}\,|$$
$$= \{\text{ if } |h| \ge 1 \text{ then } \sqrt{|h|} \text{ else } |h|/(1 + \sqrt{1-|h|})\,\} \qquad \text{(even if } h \text{ is complex)}$$

to the last estimate of δz above to deduce that, roughly,

when $2\,|\delta\mathrm{f}| \ge |\,f'(z)^2/f''(z)\,|$ then $|\delta z| \le \sqrt{(2\,|\,\delta\mathrm{f}/f''(z)\,|)}$; otherwise (and usually)
when $2\,|\delta\mathrm{f}| \le |\,f'(z)^2/f''(z)\,|$ then $|\delta z| \le 2\,|\delta\mathrm{f}/f'(z)|/\big(1 + \sqrt{(1 - 2\,|\,f''(z)\,\delta\mathrm{f}/f'(z)^2\,|)}\big)$.

…

Digression to prove the alleged inequality

$$|\,h/(1 + \sqrt{1-h})\,| \le |h|/|\,1 + \sqrt{1-|h|}\,|$$
$$= \{\text{ if } |h| \ge 1 \text{ then } \sqrt{|h|} \text{ else } |h|/(1 + \sqrt{1-|h|})\,\} \quad \text{even if } h \text{ is complex.}$$

Our task will be done if we can demonstrate why $|\,1 + \sqrt{1-|h|}\,| \le |\,1 + \sqrt{1-h}\,|$. Squaring both sides reduces our task to proving that $2\cdot\mathrm{Re}\{\sqrt{1-|h|}\} + |1 - |h|| \le 2\cdot\mathrm{Re}\{\sqrt{1-h}\} + |1-h|$. Because $|1 - |h|| \le |1-h|$, our task will be done if we prove $\mathrm{Re}\{\sqrt{1-|h|}\} \le \mathrm{Re}\{\sqrt{1-h}\}$. Both sides of this inequality are nonnegative because $\sqrt{\dots}$ is the *Principal* square root, so squaring both sides reduces our task to proving that $1 - |h| + |1 - |h|| \le 1 - \mathrm{Re}\{h\} + |1-h|$. This inequality follows from $|1 - |h|| \le |1-h|$ and $\mathrm{Re}\{h\} \le |h|$. End of proof.

The two sides of the inequality just proved can never be extremely different. We have just proved that their ratio RHS/LHS = $r(h) := |\,1 + \sqrt{1-h}\,|/|\,1 + \sqrt{1-|h|}\,| \ge 1$ for all complex h . Actually the inequalities $1 \le r(h) \le r(-1) = 1 + \sqrt{2} \approx 2.41421356\dots$ can be proved by treating the cases $|h| \le 1$ and $|h| \ge 1$ separately.

To see what happens to our overestimates of $|\delta z|$ when the gap Δz between two zeros of f becomes tiny, substitute the approximation $f'(z) \approx f''(z)\,\Delta z/2$ (do you see how to justify it?) to get two expressions

if $|\Delta z| \le 2\sqrt{2\cdot|\delta f/f''(z)|}$ then $|\delta z| \le \sqrt{2\cdot|\delta f/f''(z)|}$; otherwise

if $|\Delta z| \ge 2\sqrt{2\cdot|\delta f/f''(z)|}$ then $|\delta z| \le 4\,|\delta f/f''(z)|/\left(|\Delta z| + \sqrt{(|\Delta z|^2 - 8\,|\delta f/f''(z)|)}\right)$.

Since $|\delta f/f''(z)|$ is normally of the order of the arithmetic's roundoff threshold, we see that the computed z 's uncertainty can grow as Δz shrinks until the computed z loses about half the figures carried during computation *unless* f is computed so accurately that $|\delta f/f''(z)|$ shrinks toward zero like Δz .

End of Digression.

Our bounds upon $|\delta z|$ are needed to stop an iteration only if it converges to z from just one side. Otherwise simpler error-bounds for a real zero z could be obtained from *Straddles* as follows:

Suppose two iterates ù and ú satisfy $|f(ù)| \ge |\delta f(ù)|$, $|f(ú)| \ge |\delta f(ú)|$ and $f(ù)\cdot f(ú) \le 0$; then surely $f(x)$ changes sign at some x between ù and ú . Thus, ù and ú straddle a zero z (or a pole) of f .

Therefore iteration should stop as soon as either …

- a sufficiently tight straddle has turned up, or
- $|f(x)|$ is not much bigger than a realistic bound upon $|\delta f(x)|$.

In the latter eventuality, our bounds upon $|\delta z|$ above roughly bound the computed zero's error.