

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 $x_n \rightarrow z$ as $n \rightarrow +\infty$, 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 $\hat{U}(x) := x - 2(f(x)/f'(x)) / (1 + \sqrt{1 - 2f''(x)f(x)/f'(x)^2})$. 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 $\sqrt{\dots}$ 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 convergence 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 $f(x) := f(x) - \delta f$ because of roundoff's intervention. Then, instead of z , the best we can expect from the program is a zero $z + \delta z$ of $f(x)$. 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 $\delta z \approx \delta f / f'(z)$. 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

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

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

$$\begin{aligned} |h / (1 + \sqrt{1-h})| &\leq |h| / |1 + \sqrt{1-h}| \\ &= \{ \text{if } |h| \geq 1 \text{ then } \sqrt{|h|} \text{ else } |h| / (1 + \sqrt{1-|h|}) \} \quad (\text{even if } h \text{ is complex}) \end{aligned}$$

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

$$\begin{aligned} \text{when } 2|\delta f| \geq |f'(z)^2 / f''(z)| \text{ then } |\delta z| &\leq \sqrt{2|\delta f / f''(z)|}; \text{ otherwise (and usually)} \\ \text{when } 2|\delta f| \leq |f'(z)^2 / f''(z)| \text{ then } |\delta z| &\leq 2|\delta f / f'(z)| / (1 + \sqrt{1 - 2|f''(z)\delta f / f'(z)^2|}). \end{aligned}$$

...

Digression to prove the alleged inequality

$$\begin{aligned} |h / (1 + \sqrt{1-h})| &\leq |h| / |1 + \sqrt{1-h}| \\ &= \{ \text{if } |h| \geq 1 \text{ then } \sqrt{|h|} \text{ else } |h| / (1 + \sqrt{1-|h|}) \} \text{ even if } h \text{ is complex.} \end{aligned}$$

Our task will be done if we can demonstrate why $|1 + \sqrt{1-|h|}| \leq |1 + \sqrt{1-h}|$. Squaring both sides reduces our task to proving that $2 \cdot \operatorname{Re}\{\sqrt{1-|h|}\} + |1 - |h|| \leq 2 \cdot \operatorname{Re}\{\sqrt{1-h}\} + |1-h|$. Because $|1 - |h|| \leq |1-h|$, our task will be done if we prove $\operatorname{Re}\{\sqrt{1-|h|}\} \leq \operatorname{Re}\{\sqrt{1-h}\}$. 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 $1 - |h| + |1 - |h|| \leq 1 - \operatorname{Re}\{h\} + |1-h|$. This inequality follows from $|1 - |h|| \leq |1-h|$ and $\operatorname{Re}\{h\} \leq |h|$. End of proof.

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

$$\begin{aligned} \text{if } |\Delta z| \leq 2\sqrt{2} \cdot |\delta f / f''(z)| \text{ then } & |\delta z| \leq \sqrt{2} \cdot |\delta f / f''(z)|; & \text{otherwise} \\ \text{if } |\Delta z| \geq 2\sqrt{2} \cdot |\delta f / f''(z)| \text{ then } & |\delta z| \leq 4 |\delta f / f''(z)| / \left(|\Delta z| + \sqrt{|\Delta z|^2 - 8 |\delta f / f''(z)|} \right). \end{aligned}$$

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 \hat{u} and \acute{u} satisfy $|f(\hat{u})| \geq |\delta f(\hat{u})|$, $|f(\acute{u})| \geq |\delta f(\acute{u})|$ and $f(\hat{u}) \cdot f(\acute{u}) \leq 0$; then surely $f(x)$ changes sign at some x between \hat{u} and \acute{u} . Thus, \hat{u} and \acute{u} 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.