Pathological Functions for Newton's Method

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In the solution of equations by numerical methods, a commonly used stopping criterion is

$$|x_{n+1} - x_n| < \varepsilon, \tag{1}$$

where x_n is the nth term of the sequence generated by the method, and $\varepsilon > 0$ is the tolerance. For a specific method, the bisection method, it is not difficult to show that criterion (1) can never fail: if (1) is satisfied, then we also have $|x_{n+1} - x^*| < \varepsilon$, where x^* is the root. However, as the widely used text in numerical analysis by Burden and Faires **[1]** points out, in general, criterion (1) can fail. The text's argument is based only on abstract considerations, namely, that there exist sequences (e.g., the partial sums of the harmonic series) for which (1) is true but which nonetheless diverge. An example of a function and numerical method generating a sequence having this property is not given.

In this paper, we derive two functions, which exhibit this "false convergence" phenomenon. The first of these has no real root, but nevertheless generates a sequence under Newton's method for which (1) is satisfied for any ε, namely, $\{\sqrt{u_n}\}$ where $u_n \in \mathbb{R}$, $u_{n+1} = u_n + 1$, and $n = 0, 1, \ldots$. Although this sequence satisfies (1), it obviously does not converge. The second function, like the first one, appears to converge where there are no roots, but it has a real root, to which Newton's method will never converge.

DERIVATION. To generate the sequence $\{\sqrt{u_n}\}$ we require a function f such that (Newton's method)

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

where $x_n = \sqrt{u_n}$, $u_{n+1} = u_n + 1$, $u \in \mathbb{R}$, and $n = 0, 1, \ldots$. Rearranging this equation and utilizing the fact that $u_{n+1} = u_n + 1$ gives the differential equation

$$f'(x_n) = \frac{df}{dx_n} = \frac{f(x_n)}{x_n - \sqrt{x_n^2 + 1}}$$

or

$$\frac{df}{f} = \frac{dx}{x - \sqrt{x^2 + 1}} = \left(-x - \sqrt{x^2 + 1}\right) dx, \tag{2}$$

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which has a particular solution

$$f(x) = \frac{c \exp\left[-\frac{1}{2}\left(x^2 + x\sqrt{x^2+1}\right)\right]}{\sqrt{x + \sqrt{x^2+1}}}, \tag{3}$$

where c is the constant of integration.
By inspection of (3), f is bounded above by ce^{-x^2} for large values of x.

We now derive a function h that has a zero at $x = 0$, but nonetheless exhibits the above pathological behavior. For h, Newton's method should generate a divergent sequence $\{x_n\}$ for every starting value other than $x_0 = 0$, but should eventually satisfy criterion (1) for sufficiently large n. Thus, for x near zero, we chose for h to behave like the function $\sqrt[3]{x}$ in that Newton's method has a repelling fixed point at zero. For large x, we chose for h to behave like the function e^{-x^2} so that the sequence generated by Newton's method will resemble the one generated for function f, and will exhibit the "false convergence" property. We therefore make h the product,

$$h(x) = \sqrt[3]{x}\,e^{-x^2},$$

which, as we will demonstrate, has the desired properties. Note that because of the way that h is defined, it is bounded below by e^{-x^2}.

PROPERTIES OF FUNCTIONS

Function f. Function f, defined by equation (3) and generating the sequence $\{\sqrt{u_n}\}$, is strictly decreasing, since the first derivative of f is

$$f'(x) = f(x)\left(-x - \sqrt{x^2+1}\right) < 0. \tag{4}$$

In the limits of $x \to -\infty$ and $x \to +\infty$, we have $f(x) \to +\infty$ and $f(x) \to 0$, respectively. To demonstrate the limit as $x \to -\infty$, consider first the limit of the exponent in (3):

$$\begin{aligned}
&\lim_{x\to-\infty} -\frac{1}{2}\left(x^2 + x\sqrt{x^2+1}\right) \\
&= \lim_{x\to-\infty} -\frac{1}{2}\left[\left(x^2 + x\sqrt{x^2+1}\right)\cdot\frac{x^2 - x\sqrt{x^2+1}}{x^2 - x\sqrt{x^2+1}}\right] \\
&= \lim_{x\to-\infty} -\frac{1}{2}\left(\frac{x^4 - x^2(x^2+1)}{x^2 - x\sqrt{x^2+1}}\right) = \lim_{x\to-\infty} \frac{1}{2}\left(\frac{x^2}{x^2 - \sqrt{x^4+x^2}}\right) = \frac{1}{4}.
\end{aligned}$$

Therefore, in the limit as $x \to -\infty$, the numerator of (3) is $ce^{1/4} > 0$. In the denominator, we have

$$\lim_{x\to-\infty} x + \sqrt{x^2+1} = \lim_{x\to-\infty} \frac{-1}{x - \sqrt{x^2+1}} = 0$$

where the limit approaches 0 from above. Hence, $\lim_{x\to-\infty} f(x) = +\infty$. The graph of f is shown in Fig. 1.

Function h. The function $h(x) = \sqrt[3]{x}\,e^{-x^2}$ has a single zero at $x = 0$, but as we will see, iteration under Newton's method can never converge to this zero unless we are lucky enough to choose $x_0 = 0$. However, if the convergence criterion $|x_{n+1} - x_n| < \varepsilon$ is used (and if none of the iterates is a critical point of h, in which

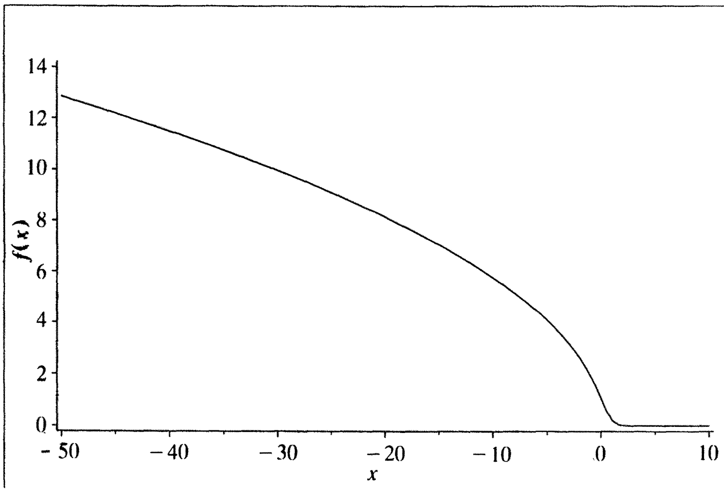

Figure 1. Function f.

case the sequnce would diverge), Newton's method will appear to converge in one of the tails of the function, i.e., where there are no zeroes.

Applying Newton's method to h yields

$$x_{n+1} = x_n - \frac{h(x_n)}{h'(x_n)} = x_n - \frac{x_n}{\frac{1}{3} - 2x_n^2} = x_n\left[1 - \frac{1}{\frac{1}{3} - 2x_n^2}\right],$$

which is defined everywhere on the real line except at the critical points of h, which are $-1/\sqrt{6}$ and $1/\sqrt{6}$.

To show that the sequence $\{x_n\}$ cannot converge to zero, consider the case when x_n is in the interval $(-1/\sqrt{6}, 1/\sqrt{6})$ and $x_n \neq 0$. We see that

$$|x_{n+1}/x_n| = \left|1 - \frac{1}{\frac{1}{3} - 2x_n^2}\right| > 2.$$

That is, instead of moving points closer to zero, this process drives them away, making each new point more than twice as far from zero as its predecessor. Clearly, this process eventually takes x_n outside the interval $(-1/\sqrt{6}, 1/\sqrt{6})$ for some n.

Now, suppose that x_k is outside of $(-1/\sqrt{6}, 1/\sqrt{6})$. We assume that x_k is in the right tail of the function, but the same properties hold for the left tail because the function is symmetric about the origin. Also, we assume that $x_k \neq 1/\sqrt{6}$, because the derivative of h at that point is zero, so Newton's method diverges.

Our convergence criterion is given as $|x_{n+1} - x_n| < \varepsilon$, which is the same thing as

$$\phi(x_n) = \frac{x_n}{2x_n^2 - \frac{1}{3}} < \varepsilon.$$

Clearly, $\phi(x_n)$ converges to zero as x_n goes to infinity, so there is some x, denoted x_c, such that for all $x_n \geq x_c$, the convergence criterion will be satisfied. To prove that x_n does get sufficiently large under iteration, we will assume that it does not and show that that leads to contradiction.

If $\phi(x_n)$ is never below ε (i.e., if x_n is never sufficiently large), then each iterate is greater than the last by at least ε. Thus, after $m > x_C/\varepsilon$ further iterations, we have

$$x_{k+m} \geq x_k + m\varepsilon > x_C.$$

This means that $\phi(x_{k+m}) < \varepsilon$, and contradicts the assumption that $\phi(x_n)$ was less than ε for no n. Thus, after sufficiently many iterations, x_n is large enough that $x_{n+1} - x_n < \varepsilon$, and the Newton's method algorithm stops, its criterion for convergence having been satisfied.

Unlike the function f, which is bounded above, $|h|$ is bounded below by e^{-x^2} for large values of x. A graph of h is shown in Fig. 2.

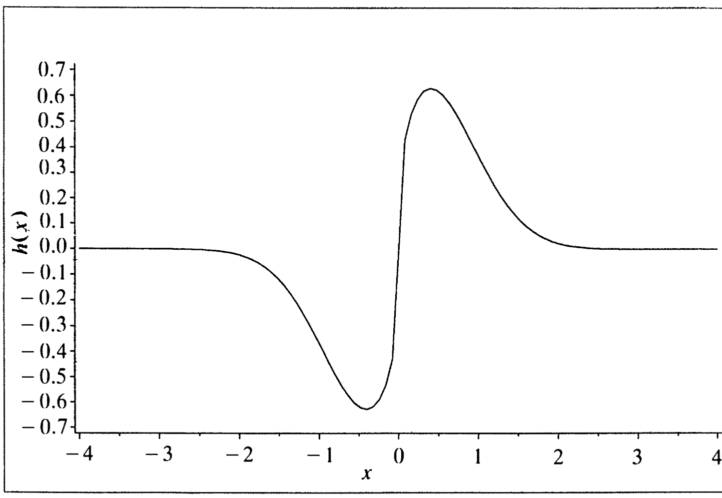

Figure 2. Function h.

THE GENERATED SEQUENCES. $\{\sqrt{u_n}\}$. Since function f in equation (3) is defined for all real numbers, any choice can be made for the initial approximation, x_0, for Newton's method. Since function f was derived to generate the sequence $\{\sqrt{u_n}\}$, where $u_{n+1} = u_n + 1$, the numerical sequence is monotone and unbounded above. If the initial approximation $x_0 \geq 0$, then letting $x_0 = \sqrt{u_0}$, we get the sequence $\{\sqrt{u_n}\}_{n=0}^{\infty}$. If $x_0 < 0$, then from the iteration formula,

$$\begin{aligned} x_{n+1} &= x_n - \frac{1}{-x_n - \sqrt{x_n^2 + 1}} \\ &= x_n - \left(x_n - \sqrt{x_n^2 + 1}\right) \\ &= \sqrt{x_n^2 + 1}\,. \end{aligned}$$

It is interesting that, because f is concave for $x_0 < 0$, the second term of the sequence is independent of the sign of the first term, x_0. Then, letting $x_1 = \sqrt{u_1}$, the remaining sequence is $\{\sqrt{u_n}\}_{n=1}^{\infty}$.

The "convergence" of the sequence is rather slow. If we used as a stopping criterion that the difference between succeeding terms be less than ε, i.e., $\sqrt{u_{n+1}} - \sqrt{u_n} < \varepsilon$, then $u_n \approx (1 - \varepsilon^2)^2/4\varepsilon^2$. As an illustration, if we let $x_0 = 1$

and $\varepsilon = 10^{-k}, k = 1, 2, 3, \ldots,$ then, neglecting round off error, the number of iterations to "convergence" would be $25 \times 10^{2(k-1)}$. In other words, to get, say, 3 decimal places of accuracy ($k = 3$) would require 250,000 iterations.

The sequence generated by h. The tails of h are very similar to the right tail of f, so the convergence of the sequence generated by h should resemble the convergence of $\{\sqrt{u_n}\}$.

Recall that for Newton's method on h, the difference between consecutive iterates is

$$\phi(x_k) = \frac{x_k}{2x_k^2 - \frac{1}{3}}.$$

This expression is unwieldy, so for simplicity, we can obtain an estimate of ϕ by neglecting the $\frac{1}{3}$. Since x_k is large for large values of k, the constant $\frac{1}{3}$ is not significant. Thus, we have,

$$\phi(x_k) \approx \frac{x_k}{2x_k^2} = \frac{1}{2x_k}. \tag{5}$$

Using this estimate, we see that $\phi(x_k) < \varepsilon$ roughly when $x_k > 1/2\varepsilon$, so we have "convergence" for any such value of x_k.

Now, if we choose a typical starting value in the right tail, say $x_0 = 1$, we can find approximate upper and lower bounds on the number of iterations required to satisfy (1) for any value of ε. By (5), each iteration step-size for x_n between 1 and 2 is at least $1/4$, so it takes at most 4 steps to get from 1 to 2. Likewise, it takes at most 6 steps to get from 2 to 3, etc. In general, the number of iterations to get from 1 to m is at most

$$\sum_{i=2}^{m} 2i = m^2 + m - 2. \tag{6}$$

Similarly, it takes at least 2 steps to get from 1 to 2, 4 steps to get from 2 to 3, etc. Thus, the number of iterations required to get from 1 to m is at least

$$\sum_{i=1}^{m-1} 2i = m^2 - m. \tag{7}$$

Substituting $1/2\varepsilon$ for m in (6) and (7), we get

$$\frac{1}{4\varepsilon^2} - \frac{1}{2\varepsilon} \leq n \leq \frac{1}{4\varepsilon^2} + \frac{1}{2\varepsilon} - 2,$$

where n is the number of iterations to "convergence."

The convergence for h is very similar to that for f. For example, to get 3 decimal places of accuracy ($\varepsilon = 10^{-3}$) would require approximately 250,000 iterations, which is what would be required for f.

As we saw above, e^{-x^2} is a bound (lower or upper) for the functions f and h for large values of x. Moreover, the three are related by the sequences generated by Newton's method. Indeed, we have already seen that the iteration function for h is

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

and it is easy to check that the iteration function for e^{-x^2} is

$$x_{n+1} = x_n + \frac{1}{2x_n} = x_n - \frac{x_n}{2x_n^2 + 0}.$$

The function f, which is given in equation (3), is approximately

$$f(x) \approx \frac{ce^{-x^2}}{\sqrt{2}x},$$

for large values of x. Using this approximation yields the iteration function:

$$x_{n+1} \approx x_n + \frac{x_n}{2x_n^2 + \frac{1}{2}}.$$

These iteration functions differ from each other only by a constant in the denominator, which becomes insignificant for large values of x_n. So under iteration by Newton's method, f, h, and e^{-x^2} all behave similarly in the tails of the functions.

CONCLUSION. Functions f and h are useful as concrete examples demonstrating that stopping criterion (1) for the solution of equations can fail. Although neither of these functions ever converges to a root, they "converge" by this criterion. Indeed, it follows that they converge by the criterion

$$\frac{|x_{n+1} - x_n|}{|x_{n+1}|} < \varepsilon, \tag{8}$$

and, because f has the limit zero as $x \to +\infty$, and h has the limit zero as $x \to \pm\infty$, they also converge by the criterion

$$|\psi(x)| < \varepsilon,$$

where ψ is f or h. Hence, the functions converge by all standard stopping criteria. However, for reasonable values of ε, convergence is very slow. Besides this pathological behavior, the functions and their generated sequences exhibit other interesting behavior: the right tails of f and h resemble the right tail of the standard normal distribution. The second term, x_1, of the sequence generated by f is independent of the sign of x_0.

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