2003/10/03 **M174 : Numerical Methods in Science and Engineering**
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§3.2 Newton's Method

Newton's method is an *iterative* method for root finding. That is, starting from some guess at the root, x_0, one iteration of the algorithm produces a number x_1, which is supposed to be closer to a root; guesses $x_2, x_3, \ldots, x_n$ follow identically.

Newton's method uses "linearization" to find an approximate root. Recalling Taylor's Theorem, we know that

$$f(x+h) \approx f(x) + f'(x)h.$$

This approximation is better when $f''(\cdot)$ is "well-behaved" between x and $x+h$. Newton's method attempts to find some h such that

$$0 = f(x+h) = f(x) + f'(x)h.$$

This is easily solved as

$$h = \frac{-f(x)}{f'(x)}.$$

An iteration of Newton's method, then, takes some guess x_k and returns x_{k+1} defined by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

An iteration of Newton's method is shown in Figure 1, along with the linearization of $f(x)$ at x_k.

Implementation Use of Newton's method requires that the function $f(x)$ be differentiable. Moreover, the derivative of the function must be known. This may preclude Newton's method from being used when $f(x)$ is a black box. As is the case for the bisection method, our algorithm cannot explicitly check for continuity of $f(x)$. Moreover, the success of Newton's method is dependent on the initial guess x_0. This was also the case with bisection, but for bisection there was an easy test of the initial interval–*i.e.*, test if $f(a_0)f(b_0) < 0$.

Our algorithm will test for goodness of the estimate by looking at $|f(x_k)|$. The algorithm will also test for neaer-zero derivative. Note that if it were the case that $f'(x_k) = 0$ then h would be ill defined.

Problems As mentioned above, convergence is dependant on $f(x)$, and the initial estimate x_0. A number of conceivable problems might come up. We illustrate them here.

Example 1. Consider Newton's method applied to the function $f(x) = \frac{\ln x}{x}$, with initial estimate $x_0 = 3$.
Note that $f(x)$ is continuous on R^+. It has a single root at $x = 1$. Our initial guess is not too far from this root. However, consider the derivative:

$$f'(x) = \frac{x\frac{1}{x} - \ln x}{x^2} = \frac{1 - \ln x}{x^2}$$

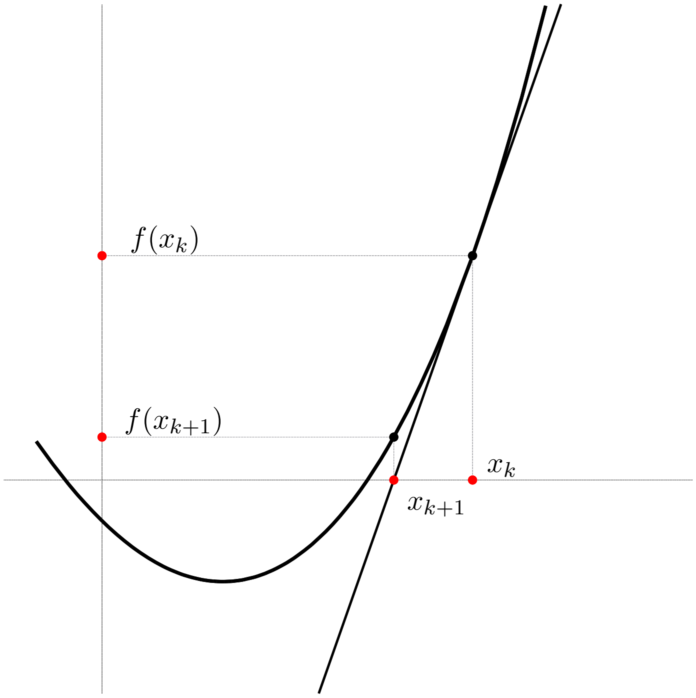

Figure 1: One iteration of Newton's method is shown for a quadratic function $f(x)$. The linearization of $f(x)$ at x_k is shown. It is clear that x_{k+1} is a root of the linearization. It happens to be the case that $|f(x_{k+1})|$ is smaller than $|f(x_k)|$, *i.e.*, x_{k+1} is a better guess than x_k.

Algorithm 1: Algorithm for finding root by Newton's Method.
Input: a function, its derivative, an initial guess, an iteration limit, and a tolerance
Output: a point for which the function has small value.

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RUN_BISECTION($f, f', x0, N, tol$)
    Let $x \leftarrow x0, n \leftarrow 0$.
    while $n \leq N$
        Let $fx \leftarrow f(x)$.
        if $|fx| < tol$
            return $x$.
        Let $fpx \leftarrow f'(x)$.
        if $|fpx| < tol$
            Warn "$f'(x)$ is small, giving up."
            return $x$.
        Let $x \leftarrow x - fx/fpx$.
        Let $n \leftarrow n + 1$.
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If $x > e^1$, then $1 - \ln x < 0$, and so $f'(x) < 0$. However, for $x > 1$, we know $f(x) > 0$. Thus taking

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} > x_k.$$

The estimates will "run away" from the root $x = 1$.

Example 2. Consider Newton's method applied to the function $f(x) = \sin(x)$ for the initial estimate $x_0 \neq 0$, where x_0 has the odious property $2x_0 = \tan x_0$.
You should verify that there are an infinite number of such x_0. Consider the identity of x_1 :

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = x_0 - \frac{\sin(x_0)}{\cos(x_0)} = x_0 - \tan x_0 = x_0 - 2x_0 = -x_0.$$

Now consider x_2 :

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -x_0 - \frac{\sin(-x_0)}{\cos(-x_0)} - x_0 + \frac{\sin(x_0)}{\cos(x_0)} = -x_0 + \tan x_0 = -x_0 + 2x_0 = x_0.$$

Thus Newton's method "cycles" between the two values $x_0, -x_0$.

Of course, Newton's method may find some iterate x_k for which $f'(x_k) = 0$, in which case, there is no well-defined x_{k+1}.

Convergence Assume that $f(x)$ has two continuous derivatives, and that it has some simple root r, *i.e.*, we assume that $f(r) = 0 \neq f'(r)$. Let $e_k = r - x_k$, the distance from x_k to the root r. Then

$$\begin{aligned} e_{k+1} &= r - x_{k+1} = r - x_k + x_k - x_{k+1}, \\ &= e_k + x_k - x_{k+1}, \\ &= e_k + \frac{f(x_k)}{f'(x_k)}, \\ &= \frac{f'(x_k)e_k + f(x_k)}{f'(x_k)}. \end{aligned}$$

Now recall Taylor's theorem, expanding about x_k:

$$0 = f(r) = f(r - x_k + x_k) = f(x_k + e_k) \quad = \quad f(x_k) + f'(x_k)e_k + \frac{f''(\xi_k)}{2}e_k^2,$$

where ξ_k is between x_k and $r = x_k + e_k$.

Then

$$e_{k+1} \quad = \quad \frac{-f''(\xi_k)e_k^2}{2f'(x_k)}.$$

Now consider the oddball function

$$c(\delta) = \frac{1}{2}\frac{\max_{|x-r|\leq\delta}|f''(x)|}{\min_{|x-r|\leq\delta}|f'(x)|},$$

for $\delta > 0$. Note that by definition $c(\delta)$ is increasing in δ, and that

$$\lim_{\delta \to 0^+} c(\delta) = \frac{1}{2}\frac{f''(r)}{f'(r)} = z.$$

By the assumption that r is a simple root, z is finite. Then there is some D such that $\delta \le D \implies \delta c(\delta) \le \frac{1}{2}$.

Now if $|r - x_k| = |e_k| < D$, then ξ_k, which is between r and x_k is also near r: $|r - \xi_k| < D$. In this case

$$\begin{aligned} |e_{k+1}| &= \left|\frac{-f''(\xi_k)}{2f'(x_k)}\right| \left|e_k^2\right|, \\ &= \left|\frac{-f''(\xi_k)}{2f'(x_k)}\right| |e_k| \, |e_k|, \\ &\le C(D) D \, |e_k| \le \frac{1}{2} |e_k| < D. \end{aligned}$$

Thus if $|e_k| < D$, then $|e_{k+1}| < D$, and so $|e_n| < D$ for $n > k$. Moreover

$$\begin{aligned} |e_{k+1}| &= \left|\frac{-f''(\xi_k)}{2f'(x_k)}\right| \left|e_k^2\right|, \\ &\le c(D) \left|e_k^2\right|. \end{aligned}$$

We term this *quadratic convergence*. That is, the error decreases quadratically. If, for example, it were the case that $c(D) = 1$, then we would double the accuracy of our root estimate with each iterate. That is, if e_0 were 0.001, we would expect e_1 to be on the order of 0.000001. The following theorem summarizes the convergence of Newton's Method.

Theorem 3 (Newton's Method Convergence). If $f(x)$ has two continuous derivatives, and r is a simple root of $f(x)$, then there is some D such that if $|x_0 - r| < D$, Newton's method will converge quadratically to r.

Suppose that $f(x)$ had another root near r, call it r'. How can we be sure that, if x_0 is sufficiently close to r, that the method converges to r, and not to the nearby r'? Hint: is $c(\delta)$ finite for all positive δ?