Solving nonlinear equations - continued

In the last lecture we presented Newton's method for solving a nonlinear equation $f(x)=0$. This method, which assumes we know a formula for the derivative $f'(x)$, is summarized as follows:

- $x_0 = \langle$ some initial guess $\rangle$
- For $k=1,2,3,\ldots$ iterate

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

We saw that Newton's method is just one example from a general family of methods, called fixed point iterations, and are defined as:

- $x_0 = \langle$ initial guess $\rangle$
- $x_{k+1} = g(x_k)$.

Newton's method is simply the fixed point iteration obtained by using $g(x) = x - \dfrac{f(x)}{f'(x)}$ as the "iteration" function.

We also discussed the following properties :

- If g is continuous, and the equation $x = g(x)$ is equivalent (subject to algebraic manipulations) to the equation $f(x) = 0$, then :

  If the sequence $\{x_k\}$ converges to the number $\underline{\underline{a}}$ then $f(a) = 0$ (i.e it is a solution)

- The sequence $\{x_k\}$ is not always guaranteed to converge. However if

$$|g(x) - g(y)| \leq L\,|x-y| \quad \text{for some } L \in [0,1)$$
$$\text{and for any } x, y \in [a,b]$$

then g will be called a <u>contraction</u>. (in $[a,b]$)

When g is a contraction on an interval $(a-\delta, a+\delta)$ around an actual solution $\underline{\underline{a}}$ to $f(x)=0$, then if x_0 (or any subsequent iterate) falls within the interval $(a-\delta, a+\delta)$, the sequence $\{x_k\}$ <u>will</u> converge to $\underline{\underline{a}}$.

- In the case where g is differentiable, an easier criterion which can be used to ensure g is a contraction, is to ensure $|g'(x)| \leq L$ $(L \in [0,1))$ with $x \in [a,b]$.

We will use these results to examine when Newton's method can be guaranteed to converge.

For Newton, we have:

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

Assume that the second derivative $f''(x)$ exists. Then:

$$g'(x) = 1 - \frac{f'(x)f'(x) - f(x)f''(x)}{[f'(x)]^2}$$

$$= \frac{f(x)f''(x)}{[f'(x)]^2}$$

We will now make some additional assumptions:

- If a is the solution $f(a)=0$, assume $f'(a) \neq 0$.
- Assume that $\lim_{x \to a} f''(x) < \infty$ (the limit exists, and it is not infinite).

Then $\lim_{x \to a} g'(x) = \frac{\overbrace{f(a)}^{=0}}{\underbrace{[f'(a)]^2}_{\neq 0}} \lim_{x \to a} f''(x) = 0.$

The fact that $\lim g'(x) = 0$ implies that we can find an interval $(a-\delta, a+\delta)$ around a, such that $g'(x)$ can be arbitrarily small. In particular for any $0 \le L < 1$ there is an appropriate δ that will guarantee that

$$\text{if } x \in (a-\delta, a+\delta) \Rightarrow |g'(x)| \le L$$

As a consequence, g will be a contraction in $(a-\delta, a+\delta)$ and, if our initial guess is in that interval, then Newton's method will converge.

In <u>some</u> cases we can estimate what the radius δ has to be, in order to guarantee convergence; we will see examples later. A good heuristic however is to evaluate $|g'(x_n)|$ during the course of the iteration. If the value is less than 1, this is a reasonable indication (but, not a proof) that the iteration is headed to convergence.

However, a simple examination of $g'(x) = \dfrac{f(x)\, f''(x)}{[f'(x)]^2}$

can give us some clues about certain cases where convergence is more likely, or more difficult to secure:

* If $f''(x) =$ small, $g'(x)$ will also tend to be small. In particular when $f''(x) = 0$ convergence is certain. Unfortunately, this is only the case for <u>linear</u> functions $f(x) = ax + b$ which are a very limited sub-case of our general nonlinear problems.

* If $f'(x)$ is large, convergence will typically occur more easily. Of course, sometimes $f' =$ large will happen at the same time $f'' =$ large, so these 2 factors will compete with one another.

Another consequence is that, when $f'(x) \approx 0$ (i.e the plot of f is mostly "flat") convergence will be quite more uncertain. Compare this with our intuitive explanation of "flat" tangents in Newton's method.

Order of convergence

We previously used the hypothesis that g is a contraction to show that $|x_k - a| \xrightarrow[k\to\infty]{} 0$. Remember that the quantity $e = x_{approximate} - x_{exact}$ was previously defined as the (absolute) error. In this case, let us define $e_k = x_k - a$ (a is the solution $f(a)=0$) as the error after the k-th iteration. If g is a contraction, we have

$$|e_{k+1}| = |x_{k+1} - a| = |g(x_k) - g(a)|$$
$$\leq L|x_k - a| = L|e_k|$$

Since $L<1$, the error shrinks at least by a constant factor at each iteration.

In some cases, we can do even better.

Remember Taylor's theorem:

If a function g has k derivatives defined, then:

$$g(y) = g(x) + g'(x)(y-x) + g''(x)\frac{(y-x)^2}{2} + g'''(x)\frac{(y-x)^3}{3!}$$
$$+ \cdots + g^{(k-1)}(x)\frac{(y-x)^{k-1}}{(k-1)!} + g^{(k)}(c)\frac{(y-x)^k}{k!}$$

Where c is a number between x & y.

For $k=1$ we simply obtain the mean value theorem:

$$g(y) = g(x) + g'(c)(y-x)$$

or $$\frac{g(y)-g(x)}{y-x} = g'(c) \quad \text{for some } c \text{ between } x \,\&\, y.$$

which we used before to show that $|g'(x)| \le L$ implies that g is a contraction with constant $= L$.

We will now use the theorem in the case $k=2$

$$g(y) = g(x) + g'(x)(y-x) + g''(c)\frac{(y-x)^2}{2}$$

Let $g = x - f/f'$ (as in Newton's method).

Also take $x = a$ (the solution) and $y = x_k$.

If $f'(a) \neq 0$ and $f''(a)$ is defined, then $g'(a) = \dfrac{\overset{=0}{f(a)}\, f''(a)}{(f'(a))^2} = 0.$

Thus, the previous equation becomes:

$$g(x_k) = g(a) + g''(c)\frac{(x_k-a)^2}{2} \quad \Rightarrow$$

$$\Rightarrow \quad x_{k+1} = a + g''(c)\,\frac{|x_k - a|^2}{2}$$

$$\Rightarrow \quad |x_{k+1} - a| = \underbrace{\frac{g''(c)}{2}}_{C_1} |x_k - a|^2$$

$$\Rightarrow \quad |e_{k+1}| \le C_1 \cdot |e_k|^2 \quad \text{← note the exponent!} \qquad (1)$$

where $C_1 = \max \left\{ \frac{g''(x)}{2} \right\}_{x \in (a, x_k)}$

Compare eq. (1) with the general guarantee

$$|e_{k+1}| \le L\,|e_k| \qquad (2) \qquad \text{for contractions:}$$

- Eq (2) depends on $L < 1$ to reduce the error.

  In Eq (1), even if C is larger, when e_k is small, then e_{k+1} will be reduced, e.g.

  $$C = 10 \qquad |e_k| = 10^{-3} \quad \Rightarrow \quad |e_{k+1}| \le 10^{-5} \ !$$

- Eq (2) implies that every iteration adds a fixed number (or fraction) of correct significant digits.

  e.g. Let $L = 0.3$

  $$|e_{k+2}| \le 0.3\,|e_{k+1}| \le 0.09\,|e_k|$$

  i.e. we gain 1 significant digit every 2 iterations.