Tuesday January 31st 2012

Solving nonlinear equations

Corresponding textbook chapter(s): §2.1,2.4

We turn our attention to the first major focus topic of our class: techniques for solving nonlinear equations. In an earlier lecture, we actually addressed one common nonlinear equation, the *quadratic* equation $ax^2 + bx + c = 0$, and discussed the potential hazards of using the seemingly straightforward quadratic solution formula. We will start our discussion with an even simpler nonlinear equation:

$$x^2 - a = 0, \quad a > 0$$

The solution is obvious, $x = \pm\sqrt{a}$ (presuming, of course, that we have a subroutine at our disposal that computes square roots). Let us, however, consider a different approach:

- Start with $x_0 = <\textit{initial guess}>$
- Iterate the sequence

$$x_{k+1} = \frac{x_k^2 + a}{2x_k} \tag{1}$$

We can show (and we will, via examples) that this method is quite effective at generating remarkably good approximations of $\sqrt{a}$ after just a few iterations. Let us, however, attempt to analyze this process from a theoretical standpoint:

If we assume that the sequence $x_0, x_1, x_2, \ldots$ defined by this method has a limit, how does that limit relate to the problem at hand? Assume $\lim x_k = A$. Then, taking limits on equation (1) we get

$$\lim x_{k+1} = \lim \frac{x_k^2 + a}{2x_k} \Rightarrow A = \frac{A^2 + a}{2A} \Rightarrow 2A^2 = A^2 + a \Rightarrow A^2 = a \Rightarrow A = \pm\sqrt{a}$$

Thus, if the iteration converges, the limit is the solution of the nonlinear equation $x^2 - a = 0$. The second question is whether it may be possible to guarantee that the described iteration *will* converge. For this, we manipulate (1) as follows

$$x_{k+1} = \frac{x_k^2 + a}{x_k} \Rightarrow x_{k+1} - \sqrt{a} = \frac{x_k^2 + a}{x_k} - \sqrt{a} = \frac{x_k^2 - 2\sqrt{a} + a}{x_k} = \frac{[x_k - \sqrt{a}]^2}{x_k}$$

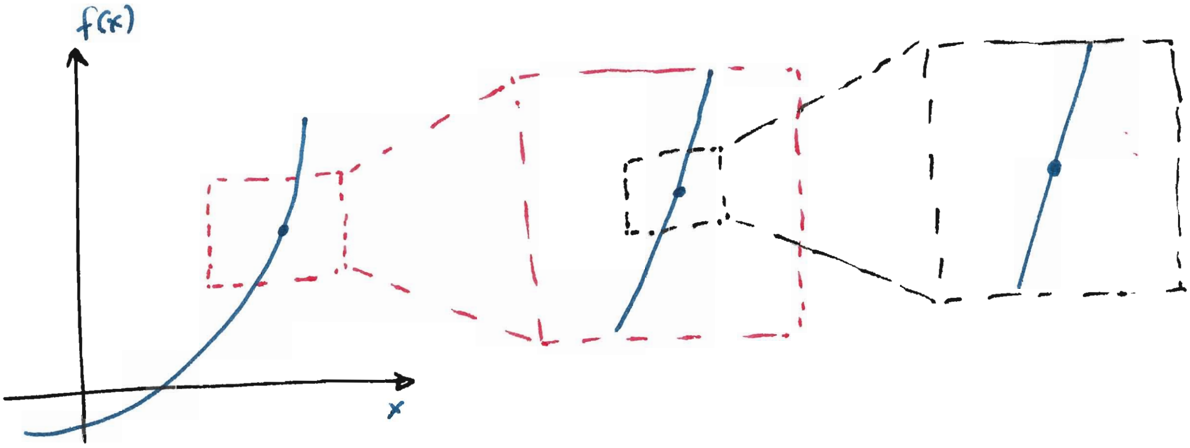
If we denote by $e_k = x_k - \sqrt{a}$ the error (or discrepancy) from the exact solution of the approximate value x_k, the previous equation reads

$$e_{k+1} = \frac{1}{x_k} e_k^2 = \frac{e_k^2}{e_k + \sqrt{a}} \tag{2}$$

For example, if we were approximating the square root of $a = 2$, and at some point we had $e_k = 10^{-3}$, the previous equation would suggest that $e_{k+1} < 10^{-6}$. One more application of this equation would yield $e_{k+2} < 10^{-12}$. Thus we see that, provided the iteration starts *close enough* to the solution, we not only converge to the desired value, but actually double the number of correct significant digits in each iteration. We defer the detailed proof until after we have introduced the more general method.

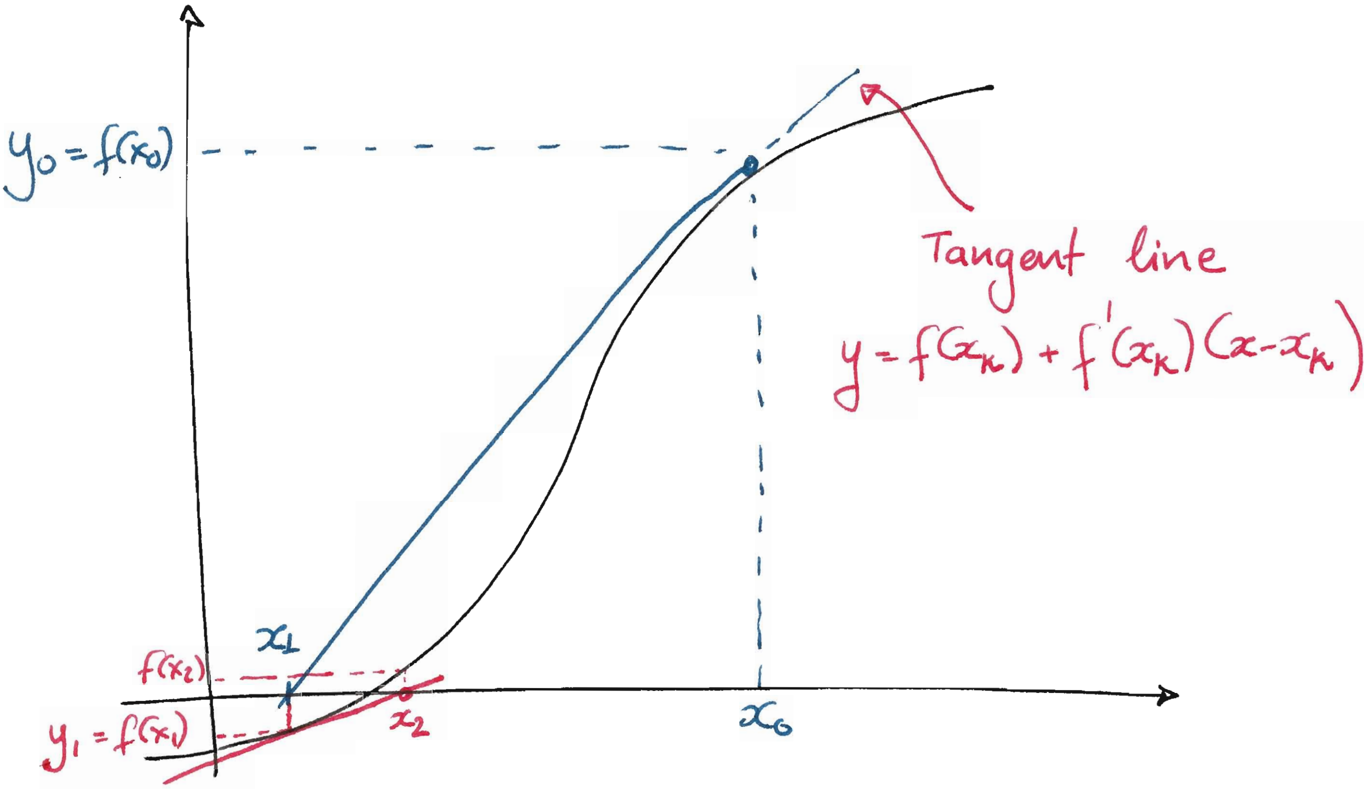
Newton's method

This example is a special case of an algorithm for solving nonlinear equations, known as Newton's method (also called the *Newton-Raphson* method). The general idea is as follows: If we "zoom" close enough to any smooth function, its graph looks more and more like a straight line (specifically, the *tangent* line to the curve).



Newton's method suggests: If after k iterations we have approximated the solution of $f(x) = 0$ (a general nonlinear equation) as x_k, then:

- Form the tangent line at $(x_k, f(x_k))$
- Select x_{k+1} as the intersection of the tangent line with the horizontal axis ($y = 0$).



If $(x_n, y_n) = (x_n, f(x_n))$, the tangent line to the plot of $f(x)$ at (x_n, y_n) is:

$$y - y_n = \lambda(x - x_n), \quad \text{where } \lambda = f'(x_n) \text{ is the slope}$$

Thus the tangent line has equation $y - y_n = f'(x_n)(x - x_n)$. If we set $y = 0$ we get:

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

Ultimately, Newton's method reduces to: $\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$

Our previous example (square root of a) is just an application of Newton's method to the nonlinear equation $f(x) = x^2 - a = 0$. Newton gives:

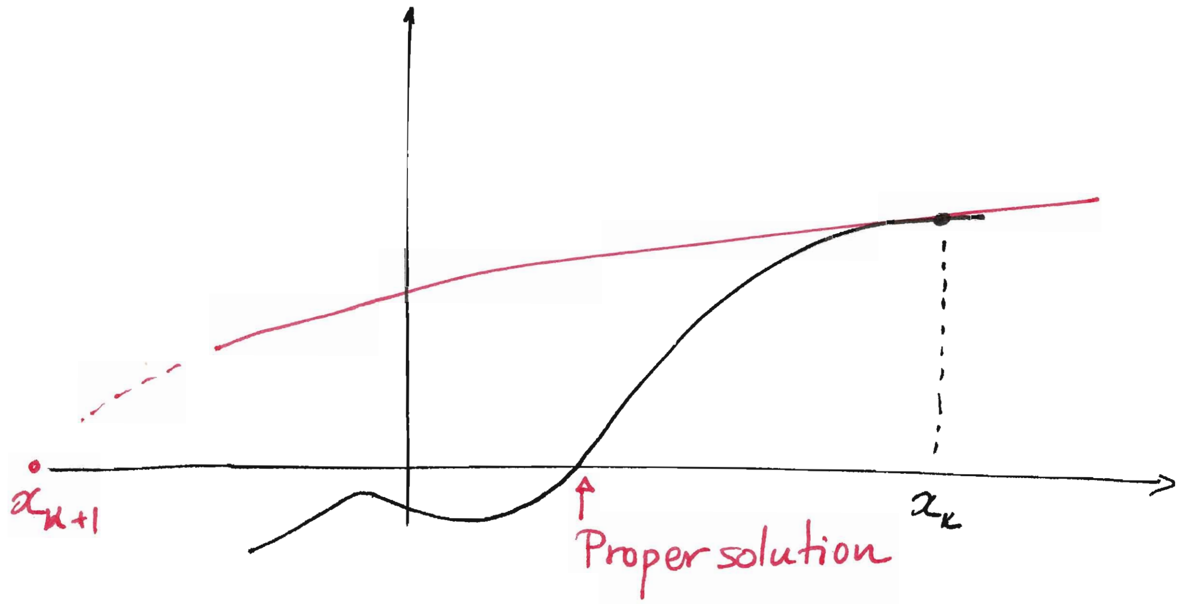
$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{x_k^2 - a}{2x_k} = \frac{2x_k^2 - x_k^2 + a}{2x_k} = \frac{x_k^2 + a}{2x_k}$$

which is the same iteration we considered previously.

A few comments about Newton's method:

- It requires the function $f(x)$ to be not only continuous, but differentiable as well. We will later see variants that do not *explicitly* required knowledge of f'. This would be an important consideration if the formula for $f'(x)$ is significantly more complex, and expensive to evaluate than $f(x)$, or in the case we simply do not possess an analytic expression for f'; this could be the case if $f(x)$ is not given to us via an explicit formula, but only defined via a black-box computer function that computes its value.

- If we ever have an approximation x_k with $f'(x_k) \approx 0$, we should expect problems, especially if we are not close to a solution (we would be nearly dividing by zero). In such cases, the tangent line is almost (or exactly) horizontal, thus the next iterate can be a very remote value, and convergence may be far from guaranteed.



Fixed point iteration

Corresponding textbook chapter(s): §2.1

Newton's method is in itself a special case of a broader category of methods for solving nonlinear equations called *fixed point iteration* methods. Generally, if $f(x) = 0$ is the nonlinear equation we seek to solve, a fixed point iteration method proceeds as follows:

- Start with $x_0 =<$ *initial guess* $>$
- Iterate the sequence

$$x_{k+1} = g(x_k)$$

where $g(x)$ is a properly designed function for this purpose. Note that $g(x)$ is related, but otherwise different than $f(x)$.

Following this method, we construct the sequence $x_0, x_1, x_2, \ldots, x_k, \ldots$ hoping that it will converge to a solution of $f(x) = 0$. The following questions arise at this point:

1. If this sequence converges, does it converge *to a solution* of $f(x) = 0$?
2. Is the iteration guaranteed to converge?
3. How fast does the iteration converge?
4. (Of practical concern) When do we stop iterating, and declare that we have obtained an acceptable approximation?

We start by addressing the first question: If the sequence $\{x_k\}$ does converge, can we ensure that it will converge to a solution of $f(x) = 0$?

Taking limits on $x_{k+1} = g(x_k)$, and assuming that (a) $\lim x_k = a$ and (b) the function g is continuous, we get:

$$\lim_{k \to \infty} x_{k+1} = \lim_{k \to \infty} g(x_k) \Rightarrow a = g(a)$$

The simplest way to guarantee that a is a solution to $f(x) = 0$ (in other words, $f(a) = 0$) is if we construct $g(x)$ such that

$$x = g(x) \text{ is mathematically equivalent to } f(x) = 0.$$

There are many ways to make this happen, e.g.

$$f(x) = 0 \Leftrightarrow x + f(x) = x \Leftrightarrow x = g(x), \quad \text{where} \quad g(x) := x + f(x)$$

or

$$f(x) = 0 \Leftrightarrow e^{-x} f(x) = 0 \Leftrightarrow e^{-x} f(x) + x^2 = x^2 \Leftrightarrow \frac{e^{-x} f(x) + x^2}{x} = x \Leftrightarrow$$

$$\Leftrightarrow g(x) = x, \quad \text{where} \quad g(x) := \frac{e^{-x} f(x) + x^2}{x}$$

or

$$f(x) = 0 \Leftrightarrow -\frac{f(x)}{f'(x)} = 0 \Leftrightarrow x - \frac{f(x)}{f'(x)} = x \Leftrightarrow g(x) = x, \quad \text{where} \quad g(x) := x - \frac{f(x)}{f'(x)}$$

The last example is exactly Newton's method; substituting the definition of $g(x)$ above into the iteration $x_{k+1} = g(x_k)$ yields the familiar Newton update equation. Thus we know that if Newton converges, it will be to a solution of $f(x) = 0$.