Introduction to Numerical Analysis I
Handout 4

1 Root finding

We consider equation $f(x) = 0$.

1.1 Iteration methods

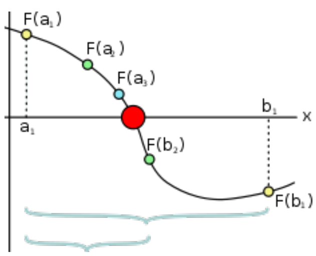
1.1.1 The Bisection Method

The idea behind the Bisection is similar to the Binary Search.

To catch a lion in the desert:

Cut the desert into two equal halves with a lion-proof fence.
Pick the half which has the lion in it and
catch the lion in that half of the desert.

Theorem 1.1. Let f be continues on $[a, b]$ and let $f(a)f(b) < 0$, then $\exists c \in (a, b)$, s.t. $f(c) = 0$.
Proof: If $f(a)f(b) < 0$ then $\operatorname{sgn}(f(a)) \neq \operatorname{sgn}(f(b))$ and therefore w.l.o.g. $f(a) < 0 < f(b)$. Thus by IVT there is $c \in (a, b)$, s.t. $f(c) = 0$.



Thus, one start with the an interval $[a, b]$ so that $f(a)$ and $f(b)$ has opposite signs and then consistently halves it, i.e. choose a subinterval $[a, c]$ or $[c, b]$, where $c = (a+b)/2$ such that f has opposite signs at the ends of the subinterval. Only one of the subintervals preserve the opposite (why?).

Definition 1.2 (The order of convergence). We say p is the order of convergence of an iterative method if

$$e_{n+1} = |r_{n+1} - \bar{r}| = c\,|r_n - \bar{r}|^p = ce_n^p$$

or, alternatively, if p is the minimal number for which

$$\lim_{n\to\infty} \frac{|r_{n+1} - \bar{r}|}{|r_n - \bar{r}|^p} = \lim_{n\to\infty} \frac{e_{n+1}}{e_n^p} = c \neq 0$$

Corollary 1.3. The bisection method has linear convergence, i.e. order of convergence $= 1$, since $e_{n+1} = 1/2\, e_n$.

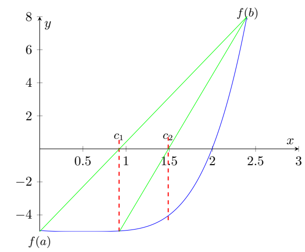
1.1.2 The Regula Falsi/False Position Method

One improves the Bisection method by reducing the interval at the intersection of the secant between $(a, f(a))$ and $(b, f(b))$

$$y = \frac{f(b) - f(a)}{b - a}(x - b) + f(b)$$

and the x-axis. Thus, the point c is now a root of the secant line Thus, instead of midpoint one uses

$$c = \frac{b(f(b) - f(a)) - f(b)(b - a)}{f(b) - f(a)} = \frac{af(b) - bf(a)}{f(b) - f(a)}$$



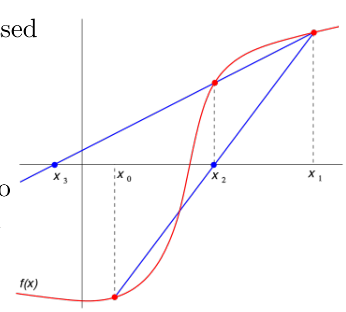
This choice of c is not better even thought c moves toward the root. There is a severe disadvantage: if the function f is convex/concave and monotonic in $[a, b]$, i.e. if $f'(x)$ and $f''(x)$ doesn't change sign, then the secant is always above/under the graph of $f(x)$, and so c is always lies to the same side from the zero. Consequently one of the ends stay fixed and the other one changes every iteration. Thus the length of the interval won't tend to zero. The sequence c_n does converge to the root, but not necessary better then bisection.

Illinois algorithm improves the problem described above. After the same end-point is retained twice in a row a modified step is used.

$$c = \frac{0.5af(b) - bf(a)}{0.5f(b) - f(a)} \quad \text{or} \quad c = \frac{af(b) - 0.5bf(a)}{f(b) - 0.5f(a)}$$

to force the next c to occur on down-weighted side of the function. Asymptotically it guarantees super-linear convergence of $p = 1.442$.

1.1.3 Secant Method



Another method based on intersection of secant and x-axis, but without an attempt to decrease interval's size. The method require two initial guesses and then use the same formula as in the Regula Falsi.

$$x_{i+1} = x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$$

If converges, the order of convergence of $p = 0.5\left(1 + \sqrt{5}\right) \approx 1.618$ (the golden ratio).

1.1.4 Newton-Raphson Iteration

Let x_k be a sequence that converges to the root of $f(x)$, i.e. $x_k \to r$ and, if f is continuous in the vicinity of r, then also $f(x_k) \to f(r) = 0$ as $k \to \infty$. Consider the Taylor expansion

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

solve it for x_{k+1}, to get the Newton's (or Newton-Raphson's) Method

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

Note that $f'(x) \approx \frac{f(x_k)-f(x_{k-1})}{x_k - x_{k-1}}$, so the Secant Method can be considered approximation of Newton's method. Although, the Secant is an older method, it was found before the derivatives were known.

The convergence of the method depends on the proximity of the initial guess to the real root. For a convergent sequence the following is true. If $f(x)$ is differentiable in the vicinity of the root r and $f'(r) \neq 0$ then the order of convergence is quadratic, i.e. $p = 2$: Let $h = |x_k - r|$

$$\frac{f(x_k)}{hf'(x_k)} = \frac{\cancel{f(r)} + hf'(r) + \frac{h^2}{2}f''(r) + O(h^3)}{h(f'(r) + hf''(r) + O(h^2))} =$$

$$\frac{f'(r) + \frac{h}{2}f''(r) + O(h^2)}{f'(r) + hf''(r) + O(h^2)} = \frac{1 + \frac{h}{2}\frac{f''(r)}{f'(r)} + O(h^2)}{1 + h\frac{f''(r)}{f'(r)} + O(h^2)} =$$

$$\frac{\left(1 + \frac{h}{2}\frac{f''(r)}{f'(r)} + O(h^2)\right)\left(1 - h\frac{f''(r)}{f'(r)} + O(h^2)\right)}{1 - \left(h\frac{f''(r)}{f'(r)} + O(h^2)\right)^2} =$$

$$\frac{1 - \overbrace{h\frac{f''(r)}{f'(r)} + \frac{h}{2}\frac{f''(r)}{f'(r)}}^{O(h)} + \alpha}{1 + O(h^2)} \to 1 + O(h),$$

where

$$\alpha = \left(\frac{h}{2}\frac{f''(r)}{f'(r)} + O(h^2)\right)\left(h\frac{f''(r)}{f'(r)} + O(h^2)\right)$$

Thus, for the smallest $p = 2$

$$\left|\frac{x_{k+1} - \bar{r}}{(x_k - \bar{r})^p}\right| = \left|\frac{x_k - \frac{f(x_k)}{f'(x_k)} - \bar{r}}{(x_k - \bar{r})^p}\right| = \left|\frac{h}{h^p} - \frac{f(x_k)}{h^p f'(x_k)}\right| =$$

$$= h^{1-p}\overbrace{\left(1 - \frac{f(x_k)}{hf'(x_k)}\right)}^{O(h)} = O(h^{2-p}) \to c \neq 0$$

Similarly one shows (in homework) that if f is twice differentiable, $f'(r) = 0$ and $f''(r) \neq 0$ then the convergence is linear.

The Chord Method To avoid extra time needed for computation of $f'(x_k)$ one attempts to evaluate it not every iteration

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_0)}$$

When the method converges the convergence is linear. A little improvement is to change $f'(x_0)$ with $f'(x_{\lfloor k/m \rfloor})$ for some integer m.

Multivariate Newton Iteration Consider $\vec{x} = (x_1, ..., x_n)$, vector function and it's Jacobian:

$$F(\vec{x}) = \begin{pmatrix} f_1(\vec{x}) \\ \vdots \\ f_n(\vec{x}) \end{pmatrix} \quad J_F = \begin{pmatrix} -\nabla f_1 - \\ \vdots \\ -\nabla f_n - \end{pmatrix}$$

The linear approximation is given by

$$F(\vec{x}_{k+1}) = F(\vec{x}_k) + J_F(\vec{x}_k) \cdot (\vec{x}_{k+1} - \vec{x}_k),$$

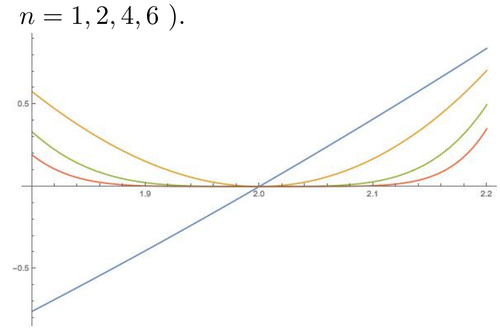
Thus, the Newton Method is reads for

$$\vec{x}_{k+1} = \vec{x_k} - J_F^{-1}(\vec{x}_k) F(\vec{x}_k)$$

1.1.5 Termination Criteria

The very important question is how to decide when to stop the iteration,

1. The criteria $|x_k - r| < \varepsilon$ or $|x_k - r|/|r| < \varepsilon$ could work, but r using assumptiion $x_k \approx r$, i.e. $|x_{k+1} - x_k| < \varepsilon$ or $|x_{k+1} - x_k|/|x_{k+1}| < \varepsilon$.
2. The criteria $f(x_k) = 0$ is problematic, due to computational errors $f(r) \neq 0$ and also often less accurate result is enough.
3. The criteria $|f(x_k)| < \varepsilon$ is wrong. When $f'(r) \approx 0$ we get $f(x_k) \approx \cancel{f(r)} + f'(r)(x_k - r) \approx$ even when $|x_k - r|$ is large. When r is multiple root the situation even worsen due to huge condition number, i.e. $\frac{1}{f'(r)} = \frac{1}{'0'}$. See the graphs of $(f(x))^n$ below for for $f(x) = x^2 - 4$ and $n = 1, 2, 4, 6$).



4. Note that $x_k - r \approx \frac{f(x_k)}{f'(r)} \approx \frac{f(x_k)}{f'(x_k)}$, thus the criteria $\left|\frac{f(x_k)}{f'(x_k)}\right| < \varepsilon$. However to use this criteria one need to compute $f'(r)$, like in Newton. Also note that in Newton this criteria is equivalent to $|x_{k+1} - x_k| < \varepsilon$.