Numerical Analysis KOM2722-AVE3842

Week 5

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Algorithm (Bisection Method)

1) Given initial interval $[a_0, b_0] = [a, b]$, set $k = 0$
2) Compute $c_{k+1} = a_k + \frac{1}{2}[b_k - a_k]$
3) If $f(c_{k+1})f(a_k) < 0$, set $a_{k+1} = a_k$, $b_{k+1} = c_{k+1}$,
4) If $f(c_{k+1})f(b_k) < 0$, set $b_{k+1} = b_k$, $a_{k+1} = c_{k+1}$
5) Update k and go to Step 2

*For very large values of a and b, $(a + b)/2$ can lead to a computational overflow, whereas $a + \frac{1}{2}(b - a)$ will not

Theorem: (Bisection Convergence and Error)

Let $[a_0, b_0] = [a, b]$ be the initial interval with $f(a)f(b) < 0$. Define the approximate root as $x_n = c_n = (b_{n-1} - a_{n-1})/2$. Then, there exists a root $\alpha \in [a, b]$ such that

$$|\alpha - x_n| \leq \left(\frac{1}{2}\right)^2 (b - a)$$

to achieve an accuracy of $|\alpha - x_n| \leq \varepsilon$

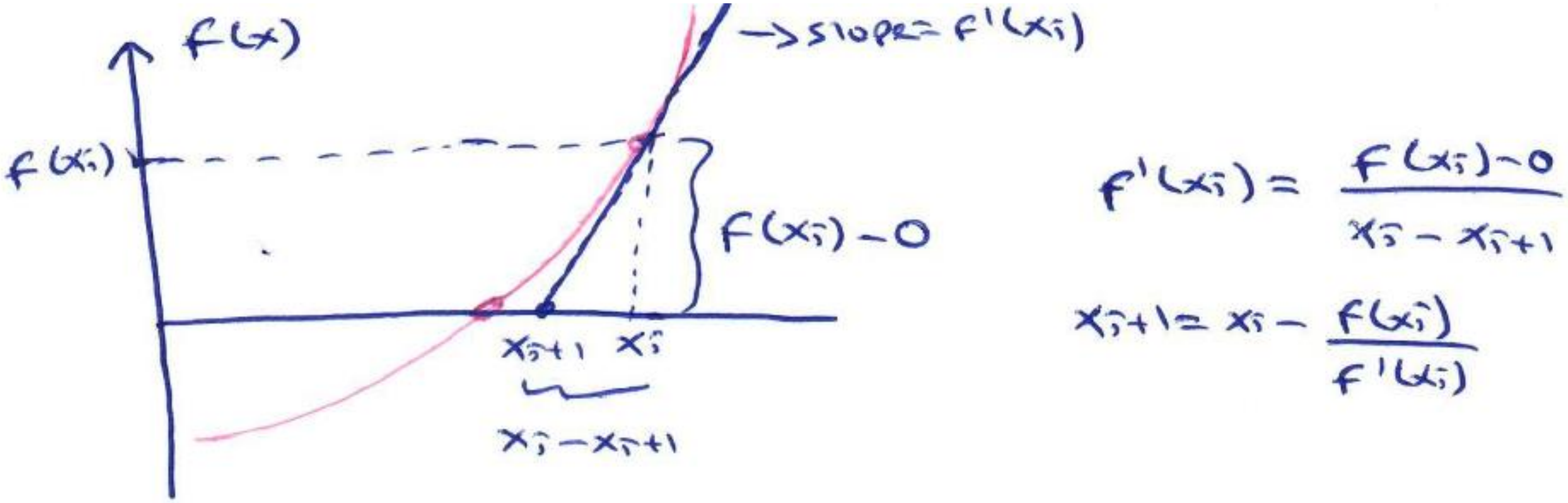
It suffices to take $n \geq \frac{\log(b-a)-\log(\varepsilon)}{\log(2)}$

Newton’s Method

The method is sometimes called Newton-Raphson, in honor of Joseph Raphson, who published the idea before Newton did.

The Newton’s method is the best-known algorithm of finding roots, it is simple and fast

The only drawback of the method is that using both the derivative $(f'(x))$ and the function itself $(f(x))$.



*If the initial guess at the root is x_i, a tangent can be extended from the point $[x_i, f(x_i)]$.

The point where this tangent crosses the x-axis usually represents an improved estimate of the root.

**The Newton-Raphson formula can be derived from Tylor series expansion of $f(x)$ about x;

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \underbrace{O(x_{i+1} - x_i)^2}_{\text{term is dropped}}$$

Assuming that x_i is close to x_{i+1},

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

Given an expression in terms of something simple plus a remainder generate a numerical approximation by dropping the remainder.

Start with x_0,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \Rightarrow x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \Rightarrow \cdots \Rightarrow x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

(draw straight lines) up to reach a close enough solution

This is Newton's Theorem based on very simple idea

->Replace a general function by a simpler function and do the required computation exactly on the simpler function

Example: $f(x) = 2 - e^x$ applying Newton's method, choose $x_0 = 0$.

$$x_1 = x_0 - \frac{2 - e^{x_0}}{-e^{x_0}} = -\frac{2-1}{-1} = 1$$

$$x_2 = x_1 - \frac{2 - e^{x_1}}{-e^{x_1}} = 1 - \frac{2-e}{-e} = 0.735758\ldots$$

$$x_3 = x_2 - \frac{2 - e^{x_2}}{-e^{x_2}} = 0.735758 - \frac{2 - e^{0.735758}}{-e^{0.735758}} = 0.694042$$

Example: A root of $f(x) = x^3 - 10x^2 + 5 = 0$ => lies close $x_0 = 0.7$ compute this root with Newton's method.

$$f'(x) = 3x^2 - 20x$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

$$x - \frac{x^3 - 10x^2 + 5}{3x^2 - 20x} = \frac{2x^3 - 10x^2 - 5}{x(3x - 20)}$$

$$x_1 = \frac{2(0.7)^3 - 10(0.7)^2 - 5}{0.7(3(0.7) - 20)} = 0.73536$$

$$x_2 = \frac{2(0.73536)^3 - 10(0.73536)^2 - 5}{0.73536(3(0.73536) - 20)} = 0.734460$$

*Newton's method is not a global method.

There are examples for which convergence will be poor or even for which convergence does NOT occur.

Usually, this can be cured by obtaining a better initial guess, it is needed to take x_0 very close to exact root (α) in order to obtain convergence.

Example: $f(x) = \frac{20x-1}{19x}, \alpha = 0.05$

$\boldsymbol{x_0}$	$\boldsymbol{x_1}$
1	-18
0.5	-4
0.25	-0.75
0.125	-0.0625
0.0625	0.046875

Example: Consider $f(x) = \arctan(x)$ -> this has a single root at 0

However, for $x_0 = 1.391745 \Rightarrow x_1 = -1.391745 \Rightarrow x_2 = 1.391745$

=>Under what conditions can we expect Newton's method to converge?

*If $f, f', and\ f''$ are continuous near the root and if f' does not equal to zero at the root, then the Newton's method will converge whenever the initial guess is sufficiently close to the root.

In this context "sufficiently close" implies that if we keep taking x_0 closer and closer to the root, we will find an x_0 such that the iteration converges.

Derivation of Newton's method from Taylor's Theorem strongly suggested

Theorem: The Newton's Error Formula

Let $f \in C^2(I)$ be given, for some interval $I \subset R$ with $f(\alpha) = 0$ for some $\alpha \in I$ for a given $x_n \in I$, define

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

Then, there exist a point ζ_n between α and x_n such that

$$\alpha - x_{n+1} = -\frac{1}{2}(\alpha - x_n)^2 \frac{f''(\zeta_n)}{f'(\zeta_n)}$$

Proof: Expanding f in a Taylor series about $x = x_n$:

$$f(x) = f(x_n) + (x - x_n)f'(x_n) + \frac{1}{2}(x - x_n)x^2 f''(\zeta_n)$$

here ζ_n is between x and α. Now set $x = \alpha$,

$$0 = f(x_n) + (\alpha - x_n)f'(x_n) + \frac{1}{2}(\alpha - x_n)^2 f''(\zeta_n)$$

Divide both sides by $f'(x_n)$, and re-arrange

$$(x_n - \alpha) - \frac{f(x_n)}{f'(x_n)} = \boxed{\frac{1}{2}(\alpha - x_n)^2 \frac{f''(\zeta_n)}{f'(x_n)}}$$

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

The error at one step goes like the square of the error at the previous step. When the error becomes small, it begins to decrease rapidly.

If we assume that convergence is occurring $(f'(\alpha) \neq 0)$ so that

$$\lim_{n\to\infty} x_n = \alpha$$

$f'(x_n) \approx f'(\alpha)$ and $f''(x_n) \approx f''(\alpha)$

$\alpha - x_{n+1} \approx -\frac{1}{2}(\alpha - x_n)^2 \frac{f''(\alpha)}{f'(\alpha)} = C(\alpha - x_n)^2$ where $C = -\frac{1}{2}\frac{f''(\alpha)}{f'(\alpha)}$

<u>Theorem:</u> Assume that f is defined and twice continuous differentiable for all x, with $f(\alpha) = 0$ for some α, define the ratio

$$M = \frac{\max_{x \in R} |f''(x)|}{2 \min_{x \in R} |f'(x)|}$$

And assume that $M < \infty$, then for any x_0 such that

$$M|\alpha - x_0| < 1$$

the Newton iteration converges, moreover

$$|\alpha - x_n| \leq M^{-1}\big(M(\alpha - x_0)\big)^{2n}$$

=> explain to us how the iteration converges.

And to assure us that if we can find a value of x_0 that is close enough to the root, then we will get convergence (a rapid convergence)

Theorem: Let $f \in C^2(I)$, where $\alpha \in I \subset R$ is a root and I is an open interval. Assume that $f'(\alpha) \neq 0$ and let the values x_n be defined by applying Newton's method to f. Then, for x_0 sufficiently close to α, we have that

$\lim_{n\to\infty} x_n = \alpha$ and $\lim_{n\to\infty} \frac{\alpha - x_{n+1}}{(\alpha - x_n)^2} = -\frac{f''(\alpha)}{2f'(\alpha)}$

The Algorithm

1) Let x be a guess for the root of $f(x) = 0$

2) Compute $\Delta x = -\frac{f(x)}{f'(x)}$

3) Let $x \leftarrow x + \Delta x$ and repeat steps 2-3 until $|\Delta x| < \varepsilon$

* Convergence can be speeded up by replacing

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

m is the multiplicity of the root. m=2 can be chosen.

The Secant Method

An obvious drawback of Newton's method is that, it requires to have a formula for the derivative of f.

There are certain function whose derivatives may be difficult or inconvenient to evaluate.

One obvious way to deal with this problem is to use an approximation to derivative in the Newton's formula.

$f'(x) \approx \frac{f(x+h)-f(x)}{h}$ -> forward difference

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

Convergence of the approximation of derivative

Reminder;

$f'(x) \approx \frac{f(x+h)-f(x)}{h}$ -> forward difference approximation

$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ -> central difference approximation

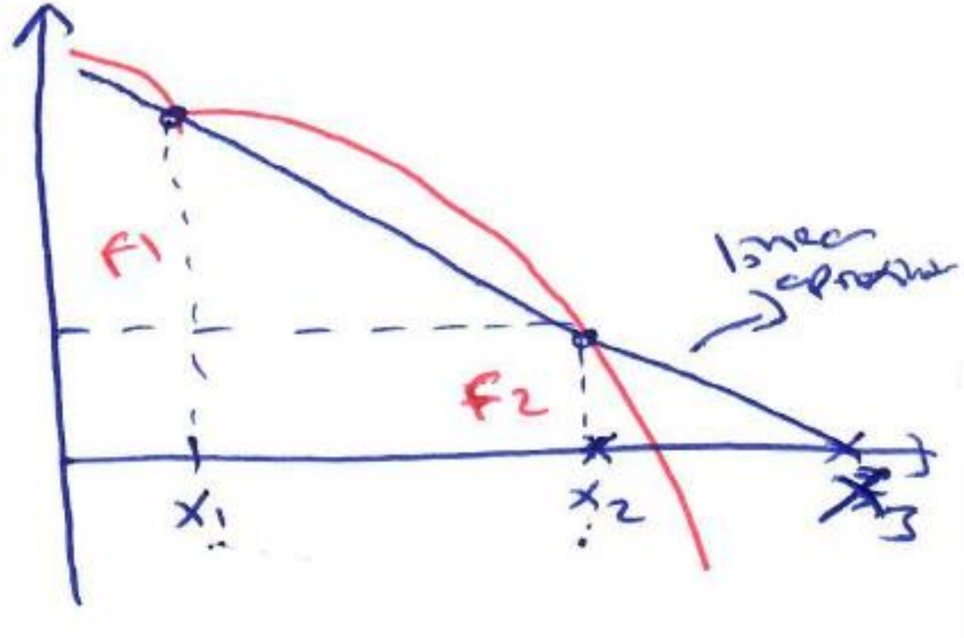
$f'(x) \approx \frac{f(x)-f(x-h)}{h}$ -> backward difference approximation

The secant method

$$x_3 = x_2 - f_2 \frac{x_2 - x_1}{f_2 - f_1}$$

More generally,

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



Example: $f(x) = 2 - e^x$, using $x_0 = 0, x_1 = 1 \Rightarrow \alpha = 0.69314718$

$$x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)} = 0.581976, \qquad error = 0.1111704$$

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)} = 0.676652, \qquad error = 0.0164544$$

$$x_4 = 0.6940813, \qquad error = 0.00093421$$

Theorem: (The Secant Method Convergence)

Let f be a twice continuously differentiable in a neighborhood of a root α, and assume that $f'(x) \neq 0$ for all x in this neighborhood. Then, for x_0 and x_1 sufficiently close to α the secant iteration converges to α with

$$\lim_{n\to\infty} \frac{\alpha - x_{n+1}}{\alpha - x_n} = 0 \text{ and } \lim_{n\to\infty} \frac{\alpha - x_{n+1}}{(\alpha - x_n)^p} = \left(\frac{1}{2}\frac{f''(\alpha)}{f'(\alpha)}\right)^{p-1}$$

For $p = \frac{1+\sqrt{5}}{2} \approx 1.618 \ldots$

** If f, f', f'' are all continuous near the root and if f' does not equal to zero at the root, then the secant method will converge whenever the initial guess is sufficiently close to the root.

Note: Evidently, the order of convergence is generally lower than for Newton's method. However, the derivatives $f'(x_n)$ need not be evaluated, and this is a definite computational advantage.

https://www.math.drexel.edu/~tolya/300_secant.pdf

Example: $f(m) = \sqrt{\frac{gm}{c_d}}\tanh\left(\sqrt{\frac{gc_d}{m}}t\right) - v(t)$ (from Book #2 page 160)

Determine the mass of the bungee jumper with a drag coefficient of 0.25 kg/m to gave a velocity 36 m/s after 4 sec of free fall. The acceleration of gravity is 9.81 m/s^2 .

Use an initial guess of 50 kg and value of 10^{-4} for perturbation fraction (desired relative error).

Fixed-Point Iteration

Consider Newton's method as applied to $f(x) = x^2 - a$

$x_{n+1} = \frac{1}{2}(x_n + \frac{a}{x_n})$ because $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

as $n \to \infty$, we know that $x_n \to \alpha = \sqrt{a}$ (In this case convergence occur for any $x_0 > 0$)

We can write more abstractly as

$$x_{n+1} = g(x_n)$$

for $g(x) = \frac{1}{2}(x + \frac{a}{x})$. Note that

$f(\alpha) = 0 <=> \alpha = g(\alpha) \Rightarrow$ This defines α, which we are ready know as the root of (the point where the graph of $y = f(x)$ crosses the x-axis), to be a point where the graph of the new function $y = g(x)$ crosses the line $y = x$

$\alpha = g(\alpha)$ shows that $g(\alpha)$ stays at $\alpha \Rightarrow$ this kind of point is called a fixed point of function g and $x_{n+1} = g(x_n) \rightarrow$ fixed-point iteration for g.

$$x^2 - \alpha = 0 \Rightarrow \alpha = g(\alpha) <=> f(\alpha) = 0 <=> \alpha = \sqrt{a}$$

* Fixed-point iteration can be developed by rearranging the function $f(x) = 0$. So that x is on the left hand side of the equation. This transformation can be accomplished either by algebraic manipulation or by simply adding x to both sided of the original equation.

Example: Suppose that we know there is a solution for the equation $x^3 - 7x + 2 = 0$ in $[0,1]$.

$$\Rightarrow x = \underbrace{\frac{1}{7}(x^3 + 2)}_{g(x)} \Rightarrow x_{n+1} = \frac{1}{7}(x_n^3 + 2)$$

Example: $f(x) = x^2 - 2x - 3 = 0 \Rightarrow$ roots at $x = -1$ and $x = 3$

- $x = g_1(x) = \sqrt{2x+3}$

If we start with $x = 4$

$$x_0 = 4, x_1 = \sqrt{11} = 3.31662, x_2 = \sqrt{9.63325} = 3.10375$$
$$x_3 = \sqrt{9.20750} = 3.03439, x_4 = \sqrt{9.06877} = 3.01144$$
$$x_5 = \sqrt{9.02288} = 3.00381$$

=> Converging on the root at $x = 3$.

- Other rearrangements of $f(x)$

$$x = g_2(x) = \frac{3}{x-2} \Rightarrow \mathrm{x}_0 = 4, \mathrm{x}_1 = 1.5, \mathrm{x}_2 = -6, \mathrm{x}_3 = -0.375,$$
$$x_4 = -1.2631, x_5 = -0.919355,$$
$$x_6 = -1.02762, x_7 = -0.990876,$$
$$x_8 = -1.00305$$

We now converge to the other root at $x = -1$,

- Consider a third rearrangement

$$x = g_3(x) = \frac{x^2-3}{2}$$

$x_0 = 4, x_1 = 6.5, x_2 = 19.625, x_3 = 191.07$ ⇒The iteration is diverging. The fixed point of $x = g(x)$ is the intersection of the line $y = x$ and $y = g(x)$ plotted against x.

** The method may converge to a root different from the expected one, or it may diverge. Different rearrangements will converge at different rates.