COURSE 12

5. Numerical methods for solving nonlinear equations in $\mathbb{R}$

Let $f : \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}$. Consider the equation

$$f(x) = 0, \quad x \in \Omega. \tag{1}$$

We attach a mapping $F : D \to D$, $D \subset \Omega^n$ to this equation.

Let $(x_0, ..., x_{n-1}) \in D$. Using F and the numbers $x_0, x_1, ..., x_{n-1}$ we construct iteratively the sequence

$$x_0, x_1, ..., x_{n-1}, x_n, ... \tag{2}$$

with

$$x_i = F(x_{i-n}, ..., x_{i-1}), \quad i = n, \ldots. \tag{3}$$

The problem consists in choosing F and $x_0, ..., x_{n-1} \in D$ such that the sequence (2) to be convergent to the solution of the equation (1).

Definition 1 *The procedure of approximation the solution of equation (1) by the elements of the sequence (2), computed as in (3), is called* F**-method.**

The numbers $x_0, x_1, ..., x_{n-1}$ *are called* **the starting points** *and the* k*-th element of the sequence (2) is called an approximation of* k*-th order of the solution.*

If the set of starting points has only one element then the F-method is **an one-step method;** if it has more than one element then the F-method is **a multistep method**.

Definition 2 *If the sequence (2) converges to the solution of the equation (1) then the* F*-method is convergent, otherwise it is divergent.*

Definition 3 *Let* $\alpha \in \Omega$ *be a solution of the equation (1) and let* $x_0, x_1, ..., x_{n-1}, x_n, ...$ *be the sequence generated by a given* F*-method. The number* p *having the property*

$$\lim_{x_i \to \alpha} \frac{\alpha - F(x_{i-n+1}, ..., x_i)}{(\alpha - x_i)^p} = C \neq 0, \quad C = constant,$$

is called the order *of the F-method.*

We construct some classes of F-methods based on the interpolation procedures.

Let $\alpha \in \Omega$ be a solution of the equation (1) and $V(\alpha)$ a neighborhood of α. Assume that f has inverse on $V(\alpha)$ and denote $g := f^{-1}$. Since

$$f(\alpha) = 0$$

it follows that

$$\alpha = g(0).$$

This way, the approximation of the solution α is reduced to the approximation of $g(0)$.

Definition 4 *The approximation of g by means of an interpolating method, and of α by the value of g at the point zero is called* **the inverse interpolation procedure.**

5.1. One-step methods

Let F be a one-step method, i.e., for a given x_i we have $x_{i+1} = F\left(x_i\right).$

Remark 5 *If $p = 1$ the convergence condition is $\left|F'\left(x\right)\right| < 1$.*

If $p > 1$ there always exists a neighborhood of α where the F-method converges.

All information on f are given at a single point, the starting value $\Rightarrow$ we are lead to Taylor interpolation.

Theorem 6 *Let α be a solution of equation (1), $V(\alpha)$ a neighborhood of α, $x, x_i \in V(\alpha)$, f fulfills the necesary continuity conditions. Then we have the following method, denoted by F_m^T, for approximating α:*

$$F_m^T(x_i) = x_i + \sum_{k=1}^{m-1} \frac{(-1)^k}{k!}[f(x_i)]^k g^{(k)}(f(x_i)), \tag{4}$$

where $g = f^{-1}$.

Proof. There exists $g = f^{-1} \in C^m[V(0)]$. Let $y_i = f(x_i)$ and consider Taylor interpolation formula

$$g(y) = (T_{m-1}g)(y) + (R_{m-1}g)(y),$$

with

$$(T_{m-1}g)(y) = \sum_{k=0}^{m-1} \tfrac{1}{k!} (y - y_i)^k \, g^{(k)}(y_i),$$

and $R_{m-1}g$ is the corresponding remainder.

Since $\alpha = g(0)$ and $g \approx T_{m-1}g$, it follows

$$\alpha \approx (T_{m-1}g)(0) = x_i + \sum_{k=1}^{m-1} \frac{(-1)^k}{k!} y_i^k g^{(k)}(y_i).$$

Hence,

$$x_{i+1} := F_m^T(x_i) = x_i + \sum_{k=1}^{m-1} \frac{(-1)^k}{k!} [f(x_i)]^k g^{(k)}(f(x_i))$$

is an approximation of α, and F_m^T is an approximation method for the solution α. ■

Particular case. For $m = 2$ we get

$$F_2^T(x_i) = x_i - \frac{f(x_i)}{f'(x_i)}.$$

This method is called **Newton's method** (**the tangent method**). Its order is 2.

Remark 7 *The higher the order of a method is, the faster the method converges. Still, this doesn't mean that a higher order method is more efficient (computation requirements). By the contrary, the most efficient are the methods of relatively low order, due to their low complexity (methods F_2^T and F_3^T).*

Newton's method

Newton's method (Newton-Raphson method) named after Isaac Newton (1642–1726) and Joseph Raphson (1648–1715), is a root-finding algorithm which produces successively better approximations to the roots of a real-valued function.

The traces of this methods can be found in ancient times (Babylon and Egypt, 1800 B.C.), as it appears in the computation of the square root of a number. This method is so efficient in computing $\sqrt{a}$, that it is a choice even today in modern codes.

According to Remark 5, there always exists a neighborhood of α where the $F-$method is convergent. Choosing x_0 in such a neighborhood allows approximating α by terms of the sequence

$$x_{i+1} = F_2^T(x_i) = x_i - \frac{f(x_i)}{f\,'(x_i)}, \quad i = 0, 1, ...,$$

with a prescribed error ε.

Lemma 8 *If $f \in C^2[a,b]$ and F_2^T is convergent, then there exists $n_0 \in \mathbb{N}$ such that*

$$|x_n - \alpha| \leq |x_n - x_{n-1}|, \quad n > n_0.$$

Remark 9 *The starting value is chosen randomly. If, after a fixed number of iterations the required precision is not achieved, i.e., condition $|x_n - x_{n-1}| \leq \varepsilon$, does not hold for a prescribed positive ε, the computation has to be started over with a new starting value.*

Another way for obtaining Newton's method.

We start with x_0 as an initial guess, sufficiently close to the α. Next approximation x_1 is the point at which the tangent line to f at $(x_0, f(x_0))$ crosses the Ox-axis. The value x_1 is much closer to the root α than x_0.

We write the equation of the tangent line at $(x_0, f(x_0))$:

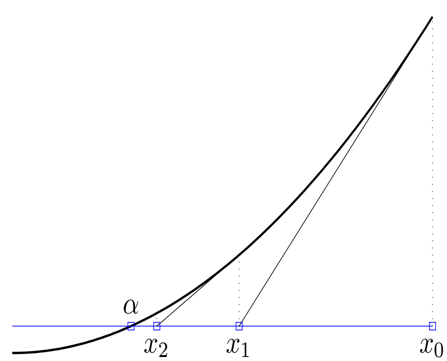
$$y - f(x_0) = f'(x_0)(x - x_0).$$

If $x = x_1$ is the point where this line intersects the Ox-axis, then $y = 0$

$$-f(x_0) = f'(x_0)(x_1 - x_0),$$

and solving for x_1 gives $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$. By repeating the process using the tangent line at $(x_1, f(x_1))$, we obtain $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$. For the general case we have

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \; n \geq 0. \tag{5}$$



The algorithm:

Let x_0 be the initial approximation; ε be a specified tolerance value; $ITMAX$ be the maximum number of iterations.

for $n = 0, 1, ..., ITMAX$

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

A stopping criterion is:

$$|f(x_n)| \leq \varepsilon \text{ or } \left|x_{n+1} - x_n\right| \leq \varepsilon \text{ or } \frac{\left|x_{n+1} - x_n\right|}{\left|x_{n+1}\right|} \leq \varepsilon.$$

Example 10 *Use Newton's method to compute a root of* $x^3 - x^2 - 1 = 0$, *to an accuracy of* 10^{-4}. *Use* $x_0 = 1$.

Sol. *The derivative of f is* $f'(x) = 3x^2 - 2x$. *Using* $x_0 = 1$ *gives* $f(1) = -1$ *and* $f'(1) = 1$ *and so the first Newton's iterate is*

$$x_1 = 1 - \frac{-1}{1} = 2 \text{ and } f(2) = 3,\ f'(2) = 8.$$

The next iterate is

$$x_2 = 2 - \frac{3}{8} = 1.625.$$

Continuing in this manner we obtain the sequence of approximations which converges to 1.465571.

5.2. Multistep methods for solving nonlinear eq. in $\mathbb{R}$

Let $f : \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}$. Consider the equation

$$f(x) = 0, \quad x \in \Omega, \tag{6}$$

We attach a mapping $F : D \to \Omega,\ D \subset \Omega^n$ to this equation.

Let $(x_0, ..., x_n) \in D$ be *the starting points*. We construct iteratively the sequence

$$x_0, x_1, ..., x_{n-1}, x_n, x_{n+1} \cdots \tag{7}$$

with

$$x_i = F\left(x_{i-n-1}, ..., x_{i-1}\right), \quad i = n+1, \ldots. \tag{8}$$

The problem consists in choosing F and $x_0, ..., x_n \in D$ such that the sequence (7) to be convergent to the solution of the equation (6).

In this case, the F-method is **a multistep method**.

It is based on interpolation methods with more than one interpolation node.

Let $\alpha \in \Omega$ be a solution of equation (6), let $(a, b) \subset \Omega$ be a neighborhood of α that isolates this solution and $x_0, ..., x_n \in (a, b)$, some given values.

Denote by g the inverse function of f, assuming it exists. Because $\alpha = g(0)$, the problem reduces to approximating g by an interpolation method with $n > 1$ nodes, for example Lagrange, Hermite, Birkhoff, etc...

Lagrange inverse interpolation

Let $y_k = f(x_k)$, $k = 0, ..., n$, hence $x_k = g(y_k)$. We attach the Lagrange interpolation formula to y_k and $g(y_k)$, $k = 0, ..., n$:

$$g = L_n g + R_n g, \tag{9}$$

where

$$(L_n g)(y) = \sum_{k=0}^{n} \frac{(y-y_0)...(y-y_{k-1})(y-y_{k+1})...(y-y_n)}{(y_k-y_0)...(y_k-y_{k-1})(y_k-y_{k+1})...(y_k-y_n)} g(y_k). \tag{10}$$

Taking

$$F_n^L(x_0, ..., x_n) = (L_n g)(0),$$

F_n^L is a $(n+1)-$ steps method defined by

$$\begin{aligned} F_n^L(x_0, ..., x_n) &= \sum_{k=0}^{n} \frac{y_0 \cdots y_{k-1} y_{k+1} \cdots y_n}{(y_k-y_0)...(y_k-y_{k-1})(y_k-y_{k+1})...(y_k-y_n)} (-1)^n g(y_k) \\ &= \sum_{k=0}^{n} \frac{y_0 \cdots y_{k-1} y_{k+1} \cdots y_n}{(y_k-y_0)...(y_k-y_{k-1})(y_k-y_{k+1})...(y_k-y_n)} (-1)^n x_k. \end{aligned}$$

Concerning the convergence of this method we state:

Theorem 11 *If* $\alpha \in (a, b)$ *is solution of equation (6),* f' *is bounded on* (a, b), *and the starting values satisfy* $|\alpha - x_k| < 1/c, \quad k = 0, ..., n$, *with* $c =$*constant, then the sequence*

$$x_{i+1} = F_n^L\left(x_{n-i}, ..., x_i\right), \quad i = n, n+1, ...$$

converges to α.

Remark 12 *The order* $ord(F_n^L)$ *is the positive solution of the equation*

$$t^{n+1} - t^n - ... - t - 1 = 0.$$

Particular case. For $n = 1$, the nodes x_0, x_1, we get **the secant method**

$$F_1^L\left(x_0, x_1\right) = x_1 - \frac{\left(x_1 - x_0\right) f\left(x_1\right)}{f\left(x_1\right) - f\left(x_0\right)},$$

Thus,

$$x_{k+1} := F_1^L\left(x_{k-1}, x_k\right) = x_k - \frac{\left(x_k - x_{k-1}\right) f\left(x_k\right)}{f\left(x_k\right) - f\left(x_{k-1}\right)}, \qquad k = 1, 2, ...$$

is the new approximation obtained using the previous approximations x_{k-1}, x_k.

The *order* of this method is the positive solution of equation:

$$t^2 - t - 1 = 0,$$

so $ord(F_1^L) = \frac{(1+\sqrt{5})}{2}$.

Comparing the Newton's method and secant method with respect to the time needed for finding a root with some given precision, we have:

-Newton's method has more computation at one step: it is necessary to evaluate $f(x)$ and $f'(x)$. Secant method evaluates just $f(x)$ (supposing that $f(x_{previous})$ is stored.)

-The number of iterations for Newton's method is smaller (its order is $p_N = 2$). Secant method has order $p_S = 1.618$ and we have that three steps of this method are equivalent with two steps of Newton's method.

- It is proved that if the time for computing $f'(x)$ is greater than ($0.44\times$the time for computing $f(x)$), then the secant method is faster.

Remark 13 *The computation time is not the unique criterion in choosing the method! Newton's method is easier to apply. If $f(x)$ is not explicitly known (for example, it is the solution of the numerical integration of a differential equation), then its derivative is computed numerically. If we consider the following expression for the numerical computation of derivative:*

$$f'(x) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} \tag{11}$$

then the Newton's method becomes the secant method.

Another way of obtaining secant method.

Based on approx. the function by a straight line connecting two points on the graph of f (not required f to have opposite signs at the initial points).

The first point, x_2, of the iteration is taken to be the point of intersection of the Ox-axis and the secant line connecting two starting points $(x_0, f(x_0))$ and $(x_1, f(x_1))$. The next point, x_3, is generated by the intersection of the new secant line, joining $(x_1, f(x_1))$ and $(x_2, f(x_2))$ with the Ox-axis. The new point, x_3, together with x_2, is used to generate the next point, x_4, and so on.

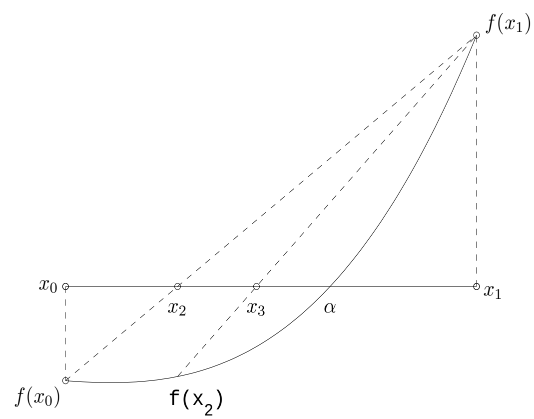
The formula for x_{n+1} is obtained by setting $x = x_{n+1}$ and $y = 0$ in the equation of the secant line from $(x_{n-1}, f(x_{n-1}))$ to $(x_n, f(x_n))$:

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

we get

$$x_{n+1} = x_n - f(x_n) \left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \right]. \tag{12}$$

Note that x_{n+1} depends on the two previous elements of the sequence $\Rightarrow$ two initial guesses, x_0 and x_1,for generating $x_2, x_3, \ldots$.



The algorithm:

Let x_0 and x_1 be two initial approximations.

for $n = 1, 2, ..., ITMAX$

$$x_{n+1} \leftarrow x_n - f(x_n)\left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right].$$

A suitable stopping criterion is

$$|f(x_n)| \le \varepsilon \text{ or } \left|x_{n+1} - x_n\right| \le \varepsilon \text{ or } \frac{\left|x_{n+1} - x_n\right|}{\left|x_{n+1}\right|} \le \varepsilon,$$

where ε is a specified tolerance value.

Example 14 *Use the secant method with $x_0 = 1$ and $x_1 = 2$ to solve $x^3 - x^2 - 1 = 0$, with $\varepsilon = 10^{-4}$.*

Sol. *With $x_0 = 1$, $f(x_0) = -1$ and $x_1 = 2$, $f(x_1) = 3$, we have*

$$x_2 = 2 - \frac{(2-1)(3)}{3-(-1)} = 1.25$$

from which $f(x_2) = f(1.25) = -0.609375$. The next iterate is

$$x_3 = 1.25 - \frac{(1.25-2)(-0.609375)}{-0.609375-3} = 1.3766234.$$

Continuing in this manner the iterations lead to the approximation 1.4655713.

Examples of other multi-step methods

1. THE BISECTION METHOD

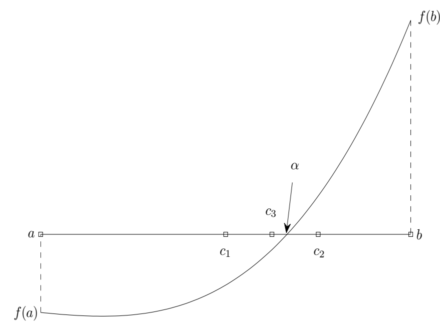
Let f be a given function, continuous on an interval $[a, b]$, such that

$$f(a)f(b) < 0. \tag{13}$$

By Mean Value Theorem, it follows that there exists at least one zero α of f in (a, b).

The bisection method is based on halving the interval $[a, b]$ to determine a smaller and smaller interval within α must lie.

First we give the midpoint of $[a, b]$, $c = (a + b)/2$ and then compute the product $f(c)f(b)$. If the product is negative, then the root is in the interval $[c, b]$ and we take $a_1 = c$, $b_1 = b$. If the product is positive, then the root is in the interval $[a, c]$ and we take $a_1 = a$, $b_1 = c$. Thus, a new interval containing α is obtained.



Bisection method

The algorithm:

Suppose $f(a)f(b) \leq 0$. Let $a_o = a$ and $b_o = b$.

for $n = 0, 1, ...,$ITMAX

$c \leftarrow \frac{a_n + b_n}{2}$

if $f(a_n)f(c) \leq 0$, set $a_{n+1} = a_n, b_{n+1} = c$

else, set $a_{n+1} = c, b_{n+1} = b_n$

The process of halving the new interval continues until the root is located as accurately as desired, namely

$$\frac{|a_n - b_n|}{|a_n|} < \varepsilon,$$

where a_n and b_n are the endpoints of the n-th interval $[a_n, b_n]$ and ε is a specified precision. The approximation of the solution will be $\frac{a_n+b_n}{2}$.

Some other stopping criterions: $|a_n - b_n| < \varepsilon$ or $|f(a_n)| < \varepsilon$.

Example 15 *The function* $f(x) = x^3 - x^2 - 1$ *has one zero in* $[1, 2]$*. Use the bisection algorithm to approximate the zero of* f *with precision* 10^{-4}*.*

Sol. *Since* $f(1) = -1 < 0$ *and* $f(2) = 3 > 0$, *then (13) is satisfied. Starting with* $a_0 = 1$ *and* $b_0 = 2$, *we compute*

$$c_0 = \frac{a_0 + b_0}{2} = \frac{1+2}{2} = 1.5 \text{ and } f(c_0) = 0.125.$$

Since $f(1.5)f(2) > 0$, *the function changes sign on* $[a_0, c_0] = [1, 1.5]$.

To continue, we set $a_1 = a_0$ *and* $b_1 = c_0$; *so*

$$c_1 = \frac{a_1 + b_1}{2} = \frac{1+1.5}{2} = 1.25 \text{ and } f(c_1) = -0.609375$$

Again, $f(1.25)f(1.5) < 0$ *so the function changes sign on* $[c_1, b_1] = [1.25,\ 1.5]$. *Next we set* $a_2 = c_1$ *and* $b_2 = b_1$. *Continuing in this manner we obtain a sequence* $(c_i)_{i>0}$ *which converges to* 1.465454, *the solution of the equation.*

2. THE METHOD OF FALSE POSITION

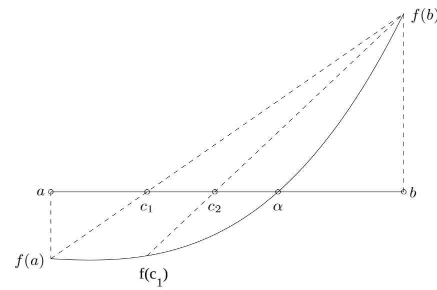
This method is also known as *regula falsi*, is similar to the Bisection method but has the advantage of being slightly faster than the latter. The function have to be continuous on $[a, b]$ with

$$f(a)f(b) < 0.$$

The point c is selected as point of intersection of the Ox-axis, and the straight line joining the points $(a,\ f(a))$ and $(b, f(b))$. From the equation of the secant line, it follows that

$$c = b - f(b)\frac{b-a}{f(b)-f(a)} = \frac{af(b)-bf(a)}{f(b)-f(a)} \qquad (14)$$

Compute $f(c)$ and repeat the procedure between the values at which the function changes sign, that is, if $f(a)f(c) < 0$ set $b = c$, otherwise set $a = c$. At each step we get a new interval that contains a root of f and the generated sequence of points will eventually converge to the root.



Method of false position.

The algorithm:

Given a function f continuous on $[a_0, b_0]$, with $f(a_0)f(b_0) < 0$,

input: a_0, b_0

for $n = 0, 1, ..., ITMAX$

$c \leftarrow \frac{f(b_n)a_n - f(a_n)b_n}{f(b_n) - f(a_n)}$

if $f(a_n)f(c) < 0$, set $a_{n+1} = a_n, b_{n+1} = c$ **else** set $a_{n+1} = c, b_{n+1} = b_n$.

Stopping criterions: $|f(a_n)| \le \varepsilon$ or $|a_n - a_{n-1}| \le \varepsilon$, where ε is a specified tolerance value.

Remark 16 *The bisection and the false position methods converge at a very low speed compared to the secant method.*

Example 17 *The function* $f(x) = x^3 - x^2 - 1$ *has one zero in* $[1, 2]$*. Use the method of false position to approximate the zero of* f *with precision* 10^{-4}*.*

Sol. *A root lies in the interval* $[1, 2]$ *since* $f(1) = -1$ *and* $f(2) = 3$*. Starting with* $a_0 = 1$ *and* $b_0 = 2$*, we get using (14)*

$$c_0 = 2 - \frac{3(2-1)}{3-(-1)} = 1.25 \text{ and } f(c_0) = -0.609375.$$

Here, $f(c_0)$ *has the same sign as* $f(a_0)$ *and so the root must lie on the interval* $[c_0, b_0] = [1.25, 2]$*. Next we set* $a_1 = c_0$ *and* $b_1 = b_0$ *to get the next approximation*

$$c_1 = 2 - \frac{3-(2-1.25)}{3-(-0.609375)} = 1.37662337 \text{ and } f(c_1) = -0.2862640.$$

Now $f(x)$ change sign on $[c_1, b_1] = [1.37662337, 2]$. Thus we set $a_2 = c_1$ and $b_2 = b_{1.}$ Continuing in this manner the iterations lead to the approximation 1.465558.

Example 18 *Compare the false position method, the secant method and Newton's method for solving the equation $x = cos x$, having as starting points $x_0 = 0.5$ și $x_1 = \pi/4$, respectively $x_0 = \pi/4$.*

n	**(a) x_n False position**	**(b) x_n Secant**	**(c) x_n Newton**
0	0.5	0.5	0.5
1	0.785398163397	0.785398163397	0.785398163397
2	0.736384138837	0.736384138837	0.739536133515
3	0.739058139214	0.739058139214	0.739085178106
4	0.739084863815	0.739085149337	0.739085133215
5	0.739085130527	0.739085133215	0.739085133215
6	0.739085133188	0.739085133215	
7	0.739085133215		

The extra condition from the false position method usually requires more computation than the secant method, and the simplifications from the secant method come with more iterations than in the case of Newton's method.

Example 19 *Consider the equation* $x^2 - x - 3 = 0$*. Give the next two iterations for approximating the solution of this equation using:*

a) Newton's method starting with $x_0 = 0$.

b) secant, false position and bisection methods starting with $x_0 = 0$ *and* $x_1 = 4$.