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Chapter 2 : Numerical Solution of Nonlinear Equations

In mathematics and applied sciences, nonlinear equations play a crucial role in modeling complex phenomena across various disciplines. Unlike linear equations, which can be solved analytically using algebraic methods, finding exact solutions for nonlinear equations is often difficult or even impossible.

For example, consider the equation :

$$\cos(x^3)\sin(2x^2-3)+0.5=0.$$

It is evident that solving this equation analytically would be extremely time-consuming, if not impossible. These types of equations, known as nonlinear (transcendental) equations, can instead be solved numerically using methods that allow us to compute approximate roots with a specified level of precision.

In this chapter, we will explore two numerical methods for solving nonlinear univariate equations of the form $f(x)=0$.

Definition 1. Any number ξ that satisfies $f(\xi)=0$ is called a solution (or root) of the equation $f(x)=0$. Geometrically, ξ represents the x-coordinate of the point where the graph of the function $f(x)$ intersects the x-axis.

Definition 2. If the equation $f(x)=0$ can be written in the form

$$f(x)=(x-\xi)^m g(x)=0$$

where $g(x)\neq 0$, then ξ is called a root of order m. If $m=1$, ξ is called a simple root of the equation $f(x)=0$.

In all iterative methods, it is necessary, to avoid divergence of the solution, to determine an interval containing the root being sought and to carefully choose the initial values.

1. Separation of Roots

Most numerical methods assume the existence of the desired root within a given interval $[a,b]$. In this case, the root is said to be localized or separated from any other potential roots.

Definition 3. We say that a root ξ of an equation $f(x)=0$ is separable if we can find an interval $[a,b]$ such that ξ is the only root of this equation in $[a,b]$. The root ξ is then called separated or localized.

the two most classical techniques for localizing or separating roots are :

Analytical method

In this case, we rely on the Intermediate Value Theorem :

Theorem 1. *Let $[a,b]\subset\mathbb{R}$ and let f be a continuous function from $[a,b]$ to $\mathbb{R}$ such that $f(a)f(b)<0$. Then there exists $\xi\in(a,b)$ such that $f(\xi)=0$.*

Example 1. Let us determine the roots of the function $f(x)=x^4-4x-1$. The variations of f are given in the following table :

x	$-\infty$		1		$+\infty$
$f'(x)$		$-$	0	$+$	
$f(x)$	$+\infty$	↘	-4	↗	$+\infty$

According to the table of variations, the function f is strictly monotonic on the intervals $[-1,0]\cup[1,2]$, with $f(-1)\cdot f(0)<0$ and $f(1)\cdot f(2)<0$. Therefore, there are two roots : $\xi_1\in(-1,0)$ and $\xi_2\in(1,2)$.

Graphical method (geometric)

Let us trace (experimentally or by studying the variations of f) the graph of the function f and look for its intersection with the Ox-axis. Alternatively, we can decompose f into two functions f_1 and f_2 that are easier to study, such that $f = f_1 - f_2$, and we search for the points of intersection of the graphs of f_1 and f_2, whose x-coordinates are exactly the roots of the equation $f(x) = 0$.

Remark 1. The functions f_1 and f_2 are often chosen with well-known graphs.

Example 2. Consider the equation

$$x \log x = 1, \quad x > 0. \tag{1}$$

This equation can also be written as : $\log x = \frac{1}{x}$. Let us define $f_1(x) = \log x$, $f_2(x) = \frac{1}{x}$, and $f(x) = f_1(x) - f_2(x) = \log x - \frac{1}{x}$. The variations of the functions f_1 and f_2 are given by the curves below (Figure 1). The x-coordinate of the point of intersection of the two curves allows us to localize the solution of the equation (1) and even provides a (first) approximation of it.

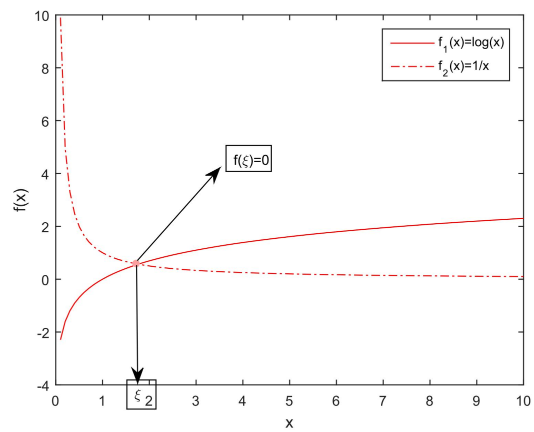

FIGURE 1: Graphical separation of the root.

2. Numerical methods for solving equations

2.1. Bisection Method

The bisection method (or dichotomy method) assumes that the function f is continuous on an interval $[a, b]$, has only one root $\xi \in (a, b)$, and satisfies $f(a)f(b) < 0$.

The principle is as follows : we set $a_0 = a$, $b_0 = b$, and define $x_0 = \frac{(a_0+b_0)}{2}$ as the midpoint of the initial interval and evaluate the function f at this point. If $f(x_0) = 0$, the point x_0 is the root of f, and the problem is solved. Otherwise, if $f(a_0)f(x_0) < 0$, the root ξ is contained within the interval (a_0, x_0), while it belongs to (x_0, b_0) if $f(x_0)f(b_0) < 0$. This process is then repeated on the new interval $[a_1, b_1]$, with $a_1 = a_0$ and $b_1 = x_0$ in the first case, or $a_1 = x_0$ and $b_1 = b_0$ in the second, and so on. In this way, we recursively construct three sequences $\{a_n\}_{n\in\mathbb{N}}$, $\{b_n\}_{n\in\mathbb{N}}$, and $\{x_n\}_{n\in\mathbb{N}}$ with :

- $x_n = \frac{a_n+b_n}{2}$
- $a_{n+1} = a_n$ and $b_{n+1} = x_n$ if $f(a_n)f(x_n) < 0$
- $a_{n+1} = x_n$ and $b_{n+1} = b_n$ if $f(x_n)f(b_n) < 0$

Proposition 1. Let f be a continuous function on the interval $[a, b]$ satisfying $f(a)f(b) < 0$. Let $\xi \in (a, b)$ be the unique solution of the equation $f(x) = 0$. Then, the sequence $\{x_n\}_{n\in\mathbb{N}}$ generated by the bisection method converges to ξ with a precision given by

$$|x_n - \xi| \leq \frac{b-a}{2^{n+1}}, \quad \forall n \in \mathbb{N}.$$

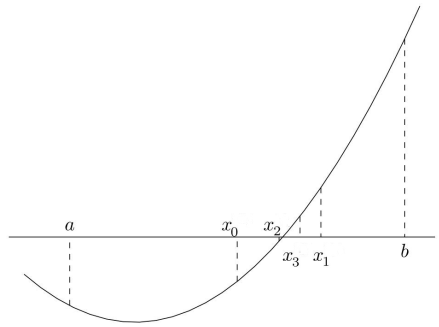

FIGURE 2: Construction of the first three iterations of the bisection method.

Remark 2. From this inequality, if the precision ε is known, the required number of iterations n can be calculated. Indeed :

$$\frac{b-a}{2^{n+1}} \leq \varepsilon \Longrightarrow n \geq \frac{\ln\left(\frac{b-a}{2\varepsilon}\right)}{\ln 2}$$

Example 3. Apply the bisection method to calculate the root of the equation $x^3+4x^2-10=0$ with a precision $\varepsilon = 10^{-2}$.
The table of variations of f is as follows :

x	$-\infty$		$-8/3$		0		$+\infty$
$f'(x)$		$+$	0	$-$	0	$+$	
$f(x)$	$-\infty$	$\nearrow$	-	$\searrow$	-10	$\nearrow$	$+\infty$

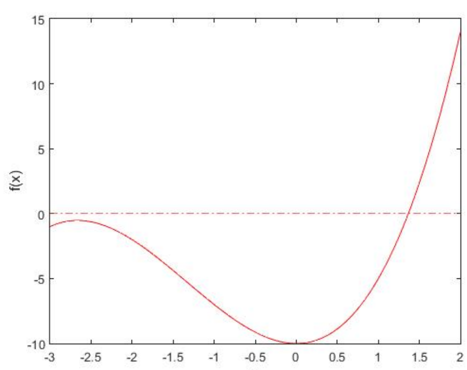

FIGURE 3: Graph of f.

From the table of variation and Figure 3, it follows that $\exists!\xi \in (1,2)$ such that $f(\xi) = 0$. Hence the required number of iterations to reach a precision of 10^-2 is

$$n \geq \frac{\ln\left(\frac{2-1}{2\times 10^{-2}}\right)}{\ln 2} \simeq 5.64$$

Then $n = 6$ and the following table summarizes the evaluated points.

n	a_n	b_n	x_n	$f(x_n)$	sign : $f(a_n).f(x_n)$	$\delta_n = \frac{b-a}{2^{n+1}}$
0	1	2	1.5	2.375	-	0.5
1	1	1.5	-1.25	-1.789	+	0.25
2	1.25	1.5	1.375	0.1621	-	0.125
3	1.25	1.375	1.3125	-0.848	+	0.0625
4	1.3125	1.375	1.3437	-0.3509	-	0.03125
5	1.3437	1.375	1.3593	-0.0964	+	0.015625
6	1.35937	1.375	1.36718	0.0322	+	0.0078125

Example 4. Let's calculate the first root of the equation $\ln(x) - x^2 + 2 = 0$ that lies in the interval $[0.1, 0.5]$ with a precision of $\varepsilon = 0.01$.
First, we calculate the number of subdivisions n to perform :

$$n \geq \frac{\ln\left(\frac{0.5-0.1}{2\times 10^{-2}}\right)}{\ln 2} \simeq 4.32 \Longrightarrow n = 5.$$

The following table summarizes the steps of the method.

n	a_n	b_n	x_n	$f(x_n)$	sign : $f(a_n).f(x_n)$	$\delta_n = \frac{b-a}{2^{n+1}}$
0	0.1	0.5	0.3	0.706	-	0.2
1	0.1	0.3	0.2	0.351	-	0.1
2	0.1	0.2	0.15	0.08	-	0.05
3	0.1	0.15	0.125	-0.095	+	0.025
4	0.125	0.15	0.1375	-0.030	+	0.0125
5	0.1375	0.15	0.14375	0.0393	-	0.0062

2.2. Newton-Raphson Method

This method is the most used for finding roots in one-dimensional problems. However, it requires the evaluation of $f(x)$ and $f'(x)$.

Let ξ be a unique root of the equation $f(x) = 0$ on the interval $[a, b]$, such that f is continuous and satisfies :

$$f'(x) \neq 0, \forall x \in [a, b], \tag{2}$$
$$f''(x) \neq 0, \forall x \in [a, b]. \tag{3}$$

The main idea of this method is to replace, at each iteration k, the arc of the curve of the function $y = f(x)$ on $[a, b]$ with the tangent to this arc at the point $(x_n, f(x_n))$: The abscissa x_{n+1} of the intersection of the tangent equation with the Ox-axis is an approximation of the unique solution ξ in $[a, b]$ for the equation $f(x) = 0$ (see Figure 4).

The equation of the tangent is :

$$y = f(x_n) + f'(x_n)(x - x_n),$$

which intersects the Ox-axis at the point $(x_{n+1}, 0)$, from which we get :

$$f(x_n) + f'(x_n)(x_{n+1} - x_n) = 0,$$

which gives the following iterative scheme (Newton-Raphson) :

$$\begin{cases} -\text{Select a starting point} x_0 \in [a, b] \text{ with} f(x_0).f''(x_0) > 0. \\ -\text{Set } x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \end{cases}$$

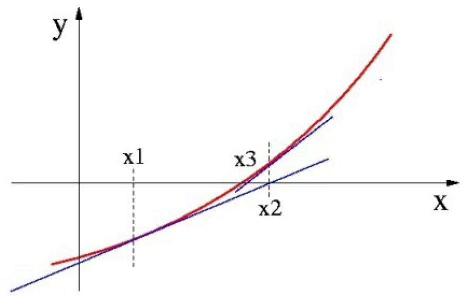

FIGURE 4: Construction of the first three iterates using Newton-Raphson method.

Proposition 2. Let f be a continuous function on the interval $[a, b]$, satisfying $f(a)f(b) < 0$, and let $\xi \in (a, b)$ be the unique solution of the equation $f(x) = 0$. If $f \in \mathcal{C}^2([a, b])$ such that for all $x \in [a, b]$, $f'(x) \cdot f''(x) \neq 0$, then the sequence $\{x_n\}_{n\in\mathbb{N}}$ constructed by the Newton-Raphson method converges to ξ with a precision given by :

$$|x_n - \xi| \leq \frac{M_2}{2m_1}(x_n - x_{n-1})^2$$

where

$$M_2 = \max_{[a,b]}\{|f''(x)|\}, \quad m_1 = \min_{[a,b]}\{|f'(x)|\}.$$

Example 5. Let's calculate the root of the function $f(x) = x^3 - x - 4$ in $[1, 2]$, within a precision of 10^{-2}, using the Newton-Raphson method.
We have $f(1) \cdot f(2) < 0$, and for all $x \in [1, 2]$, $f'(x) = 3x^2 - 1 > 0$ and $f''(x) = 6x > 0$. We have

Applying the iterative scheme of the Newton-Raphson algorithm starting from $x_0 = 2$ with $f(2) \cdot f''(2) > 0$, we get :

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 2 - \frac{f(2)}{f'(2)} = 1.8181,$$
$$|\xi - x_1| \leq \frac{M_2}{2m_1}(x_1 - x_0)^2 = \frac{12}{2 \times 2}(1.818 - 2)^2 \approx 0.01,$$

where

$$M_2 = \max_{[1,2]}\{|f''(x)|\} = f''(2) = 12 \quad \text{and} \quad m_1 = \min_{[1,2]}\{|f'(x)|\} = f'(1) = 2,$$

Next, for x_2 :

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 1.8181 - \frac{f(1.8181)}{f'(1.8181)} = 1.7966,$$
$$|\xi - x_2| \leq \frac{M_2}{2m_1}(x_2 - x_1)^2 = \frac{12}{4}(1.7966 - 1.818)^2 \approx 0.001 < 0.01.$$

Thus, $\xi = 1.7966 \pm 0.001$.

In some situations, the derivative f' can be quite complicated, or even impossible to calculate. In this case, we approximate the derivative of f using a rate of change. This method is called the **secant method** :

$$\begin{cases} -\text{Select } x_0, x_1 \in [a, b] \text{ close to } \xi. \\ -\text{Set } x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}. \end{cases}$$

Here, x_{n+1} depends on both x_n and x_{n-1} : we say that it is a **two-step method** ; indeed, we need two initial iterates, x_0 and x_1. The advantage of this method is that it does not require the calculation of the derivative f'. The drawback is that the convergence is no longer as fast.