# Numerical Methods

## Introduction to Numerical Methods

What is mean by NUMERICAL METHODS ?

Why do we need them?

Topics covered in 19MAT201.

**Numerical Methods:**
Algorithms that are used to obtain numerical solutions of a mathematical problem.

**Why do we need them?**

1.No analytical solution exists ( $5x+1=e^{-x}$, $2x+1=x\sin(x)$, $x^9-2x^2+5=0$ etc., )

2. An analytical solution is difficult to obtain or not practical.

3. Many theoretical approaches involve a numerical evaluation of resulting equations as a final step. Hence, success of a theory often depends crucially on the feasibility of its numerical evaluation.

4. Nearly all measurable quantities in real materials are off limits for analytical computation. If you want to compare a theory to experiment, numerical methods are needed to account for the complexity of chemical interactions, real lattice structures, interplay of various phenomena present at the same time, and so on.

**Note**: “No analytical solution" is not the same as unsolvable. An analytic solution is just one that can be represented in a certain way (a finite combination of certain well-known functions and constants).
Often it is the case we can prove the non-existence of analytical solutions, such as an antiderivative xtan(x) or exp($x^2$). But they're certainly solvable in the sense that we can prove the solution exists and we can compute them to any degree of accuracy.

## What do we need?

Basic Needs in the Numerical Methods:

- Practical:

Can be computed in a reasonable amount of time.

- Accurate:

Good approximate to the true value,
Information about the approximation error
(Bounds, error, order,... ).

# Types of Numerical Methods

- There are many types of numerical methods. Of them the most commonly used ones may be cited as below;

1. Methods of finding the roots of an equation. They include, bisection method, Regula Falsi method, Secant method, Newton’s method & Fixed-point iteration method.
2. Methods of solving the system of linear algebraic equations.
3. Interpolation.
4. Numerical Differentiation.
5. Numerical Integration.
6. Solution of differential equation.
7. Solution of matrix problems.
8. Solution of boundary value problem.

**Numerical Solution of Algebraic and Transcendental Equations:**

## Objective is to find a solution of $f(x)$ = 0.

An expression of the form $f(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n, a_0 \neq 0$ is called a polynomial of degree '$n$' and the equation $f(x)$ = 0 is called an **algebraic equation** of $nth$ degree.

Example for algebraic equations:
$x^9 - 2x^2 + 5 = 0$ , $x^3 - 2x^2 + 5 = 0$, $2x^2 + 5x + 1 = 0$ .

If $f(x)$ = 0 contains trigonometric, logarithmic or exponential functions, then $f(x)$ = 0 is called a **transcendental equation**.

Example for transcendental equation:
$5x + 1 = e^{-x}$ , $2x + 1 = x\sin(x)$ .
If $f(x)$ is an algebraic polynomial of degree less than or equal to 4, direct methods for finding the roots of such equation are available. But if $f(x)$ is of higher degree or it involves transcendental functions, direct methods do not exist and we need to apply numerical methods to find the roots of the equation $f(x)$ = 0.

**Some basic useful results:**

1. If $\alpha$ is root/solution of the equation $f(x)$ = 0, then $f(\alpha)$ = 0.

2. Every equation of $nth$ degree has exactly $n$ roots (real or imaginary).

3. **Intermediate Value Theorem**: If $f(x)$ is a continuous function in a closed Interval $[a, b]$ and $f(a)$ & $f(b)$ are having opposite signs, then the equation $f(x)$ = 0 has atleast one real root or odd number of roots between $a$ and $b$.

4. If $f(x)$ is a continuous function in the closed interval $[a,b]$ and $f(a)$ & $f(b)$ are of same signs, then the equation $f(x)$ = 0 has no root or even number of roots between $a$ and $b$.

**Some basic useful results:**

**Theorem:** An equation f(x)=0, where f(x) is a real continuous function, has at least one root between a and b if f(a) f(b) < 0.

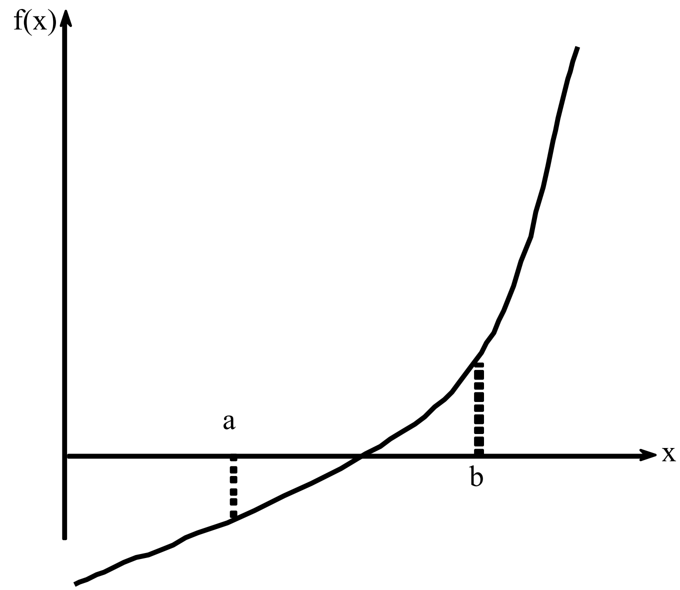
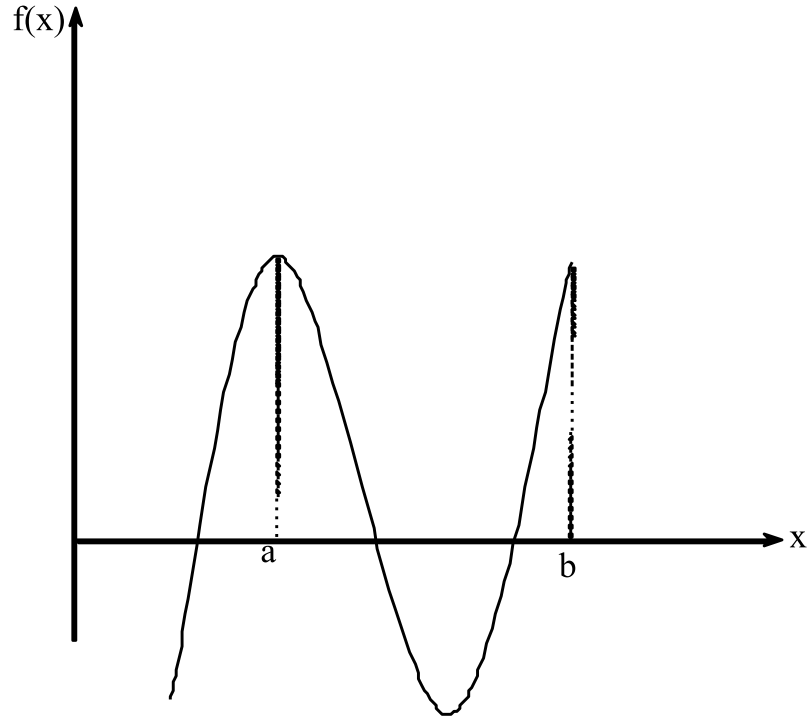



**Figure :** At least one root exists between the two points if the function is real, continuous and changes sign.

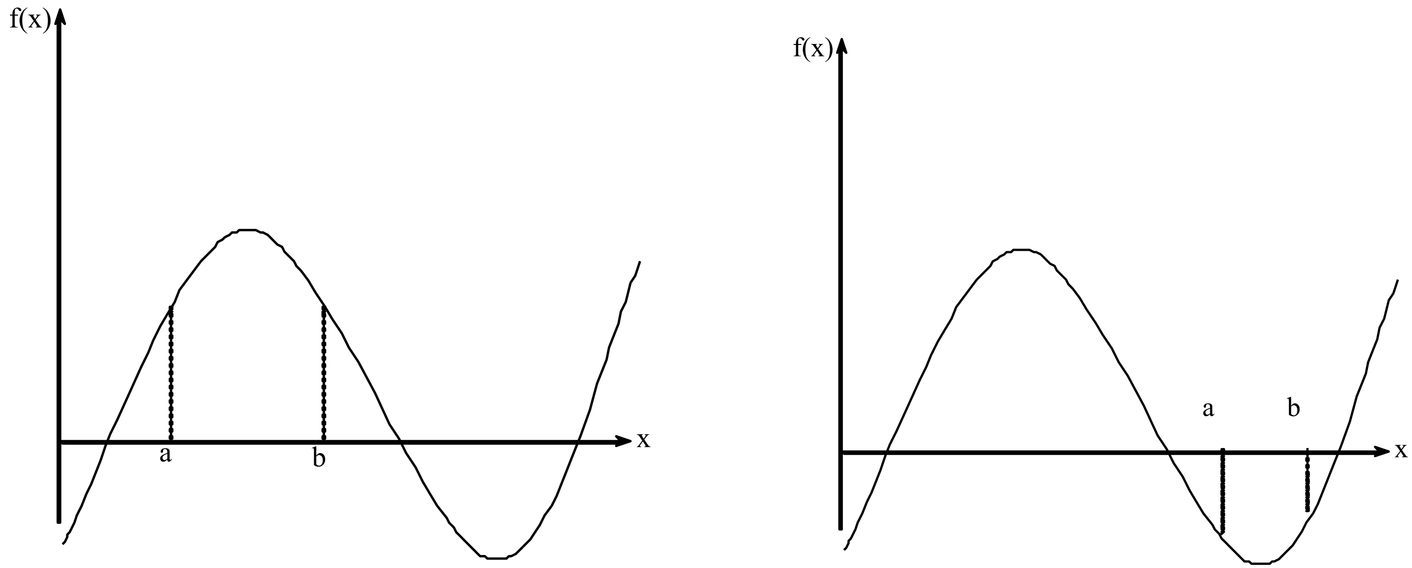
**Some basic useful results:**

Now, we discuss about the existence/non-existence of root to the given equation for the choice of a and b.(Assume f is continuous)



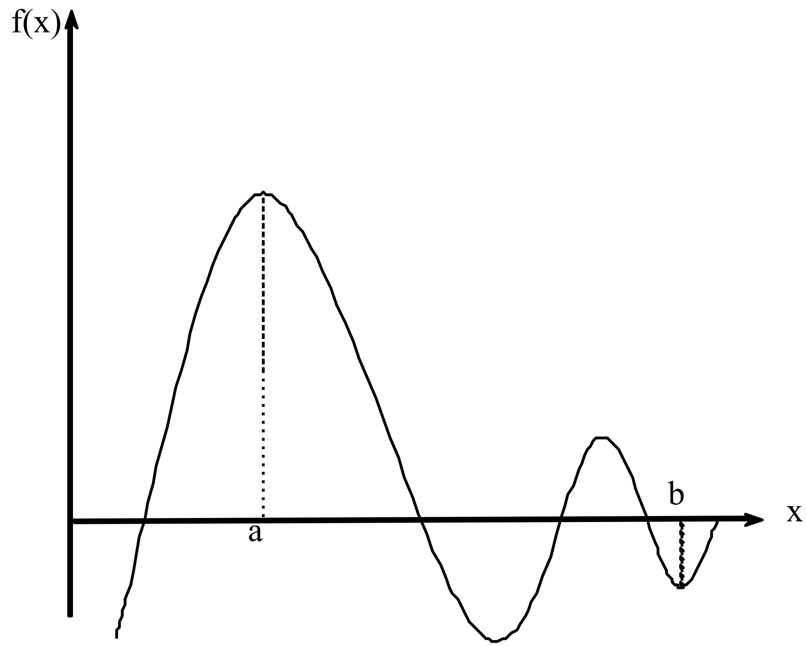

If function f(x) does not change sign between two points, roots of the equation f(x) may still exist between the two points.

**Some basic useful results:**




If the function f(x) does not change sign between two points, there may not be any roots for the equation f(x) between the two points.

**Some basic useful results:**




If the function f(x) changes sign between two points, more than one root for the equation f(x) may exist between the two points.

To find a root of the given equation, we have following methods:

Bisection method

Regula Falsi method (or) False position method

Newton’s method (or) Newton-Raphson’s Method

Secant method

Fixed-point iteration method.

# Bisection Method:

**Algorithm**:

Let $f(x)$ be a continuous function in the interval $[a, b]$ , such that $f(a)$ and $f(b)$ are of opposite signs, i.e. $f(a)\ f(b) < 0$.

Step1. Take the initial approximation given by $x_0 = (a + b)/2$ , one of the three conditions arises for finding the 1st approximation $x_1$

1. $f(x_0) = 0$, we have a root at $x_0$.

2. If $f(a)f(x_0) < 0$, the root lies between $a$ and $x_0$

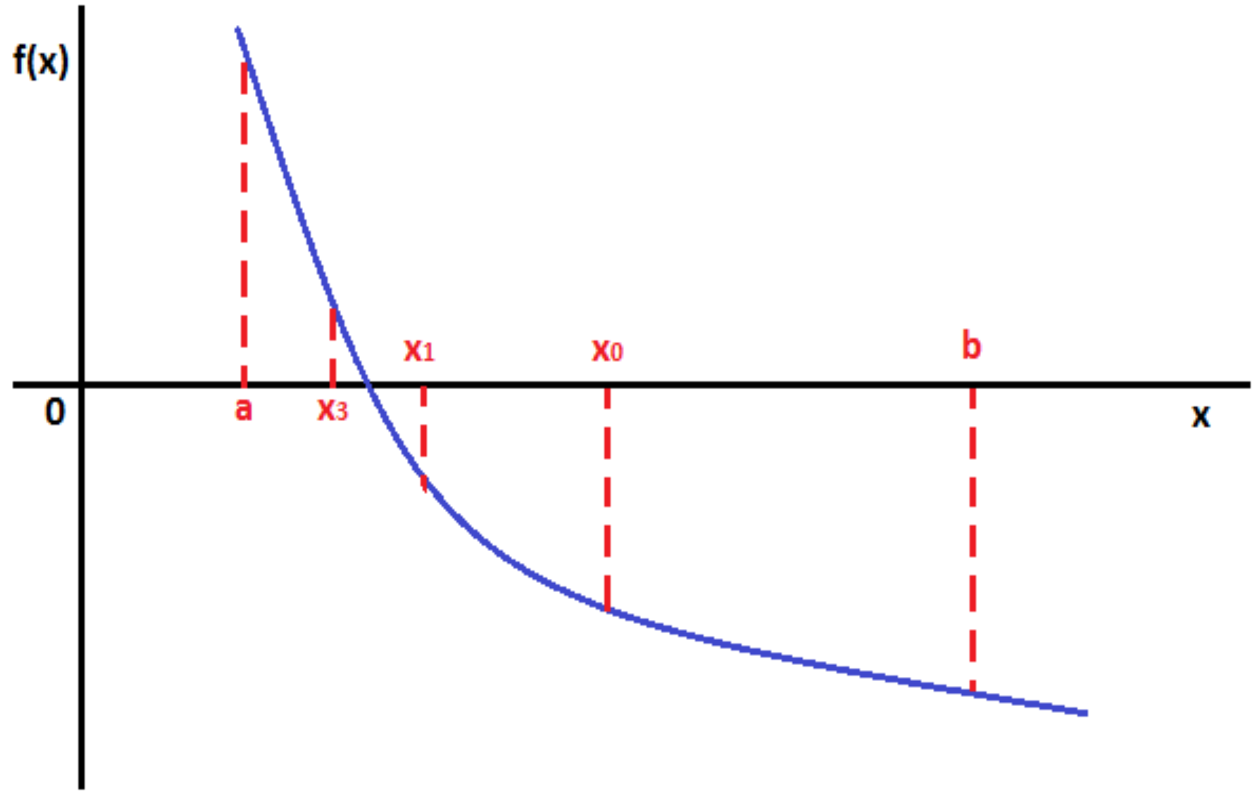
$\therefore\ x_1 = (a + x_0)/2$ and repeat the procedure by halving the interval again.

3. If $f(b)f(x_0) < 0$ , the root lies between $x_0$ and $b$

$\therefore\ x_1 = (b + x_0)/2$ and repeat the procedure by halving the interval again.

4. Continue the process until root is found to be of desired accuracy.

**The graph of Bisection Method:**



**Example1** Apply bisection method to find a root of the equation $x^4 + 2x^3 - x - 1 = 0$

(correct to two decimal places. )

**Solution:** $f x = x^4 + 2x^3 - x - 1$

Here $f(0) = -1$ and $f(1) = 1 \Rightarrow f(0)f(1) < 0$

Also $f\ x$ is continuous on[0,1], $\therefore$ atleast one root exists in [0,1].

| Iteration | a | b | $x_n$ | $f(x_n)$ |
|---|---|---|---|---|
| 0 | 0 | 1 | 0.5 | −1.1875 |
| 1 | 0.5 | 1 | 0.75 | −0.5898 |
| 2 | 0.75 | 1 | 0. 875 | 0.051 |
| 3 | 0.75 | 0.875 | 0.8125 | −0.30394 |
| 4 | 0.8125 | 0.875 | 0.84375 | −0.135 |
| 5 | 0.84375 | 0.875 | 0.8594 | −0.0445 |
| 6 | 0.8594 | 0.875 | **0.8672** | 0.0027 |
| 7 | 0.8594 | 0.8672 | **0.8633** | 0.0210 |

First two decimal places have been stabilized; hence **0.8633** is the real root correct to two decimal places.

**Example 2** Apply bisection method to find a root of the equation $x^3 - 2x^2 - 4 = 0$ correct to three decimal places.

Here $f(2) = -4$ and $f(3) = 5 \Rightarrow f(2)\, f(3) < 0$

Also $f x$ is continuous on [2,3] . $\therefore$ atleast one root exists in [2,3].

| Iteration | a | b | $x_n$ | $f(x_n)$ |
|---|---|---|---|---|
| 0 | 2 | 3 | 2.5 | −1.8750 |
| 1 | 2.5 | 3 | 2.75 | 1.6719 |
| 2 | 2.5 | 2.75 | 2.625 | 0.3066 |
| 3 | 2.5 | 2.625 | 2.5625 | −0.3640 |
| 4 | 2.5625 | 2.625 | 2.59375 | −0.0055 |
| 5 | 2.59375 | 2.625 | 2.60938 | 0.1488 |
| 6 | 2.59375 | 2.60938 | 2.60157 | 0 .0719 |
| 7 | 2.59375 | 2.60157 | 2.59765 | 0 .0329 |
| 8 | 2.59375 | 2.59765 | 2.5957 | 0.0136 |
| 9 | 2.59375 | 2.5957 | 2.5947 | −0.004 |
| 10 | 2.5947 | 2.5957 | 2.5952 | −0.0011 |
| 11 | 2.5952 | 2.5957 | 2.5955 | 0.0112 |

Hence 2.5955 is the real root correct to three decimal places.

**Example 3** Using bisection method find an approximate root of the equation $\sin(x) = 1/x$ correct to two decimal places.

**Solution:** $f(x)= x\sin(x) - 1$

Here $f(1)= \sin 1 - 1 = -0.1585$ and $f(2)= 2\sin 2 - 1 = 0.8186$

Also $f(x)$ is continuous on $[1,2]$, $\therefore$ atleast one root exists in $[1,2]$.

| Iteration | a | b | $x_n$ | $f(x_n)$ |
|---|---|---|---|---|
| 0 | 1 | 2 | 1.5 | 0.4963 |
| 1 | 1 | 1.5 | 1.25 | 0.1862 |
| 2 | 1 | 1.25 | 1.125 | 0.0151 |
| 3 | 1 | 1.125 | 1.0625 | −0.0718 |
| 4 | 1.0625 | 1.125 | 1.09375 | −0.0284 |
| 5 | 1.09375 | 1.125 | 1.10937 | −0.0066 |
| 6 | 1.10937 | 1.125 | 1.11719 | 0.0042 |
| 7 | 1.10937 | 1.11719 | 1.11328 | −0.0012 |

Hence 1.11328 is the real root correct to two decimal places.

**Advantages of bisection method :**

a) The bisection method is always convergent. Since the method brackets the root, the method is guaranteed to converge.

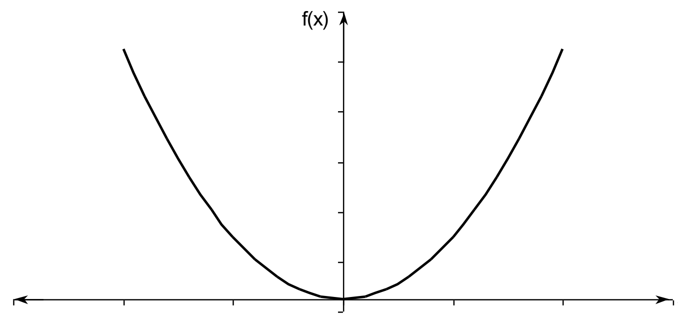
b) As iterations are conducted, the interval gets halved. So one can guarantee the error in the solution of the equation.

**Disadvantages of bisection method :**

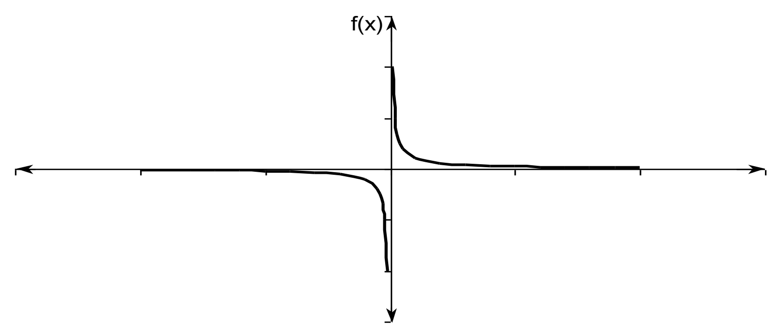
a) The convergence of the bisection method is slow as it is simply based on halving the interval.

b) If one of the initial guesses is closer to the root, it will take larger number of iterations to reach the root.

c) If a function f(x) is such that it just touches the x-axis it will be unable to find the lower and upper guesses (Ex: f(x)= $x^2$)




d) Function changes sign but root does not exist(Ex: f(x)=1/x, x is not equal to 0.)



**Exercise Problems:**

1. Calculate the first 3 iterations of the Bisection method on $x^3 - 7x^2 + 14x - 6 = 0$ with the following starting intervals

i)[0,1]

ii)[2.5,3.2]

iii)[3.2,4]

2. Apply bisection method to find a root of the equation $xe^x = 1$ correct to three decimal places

3. Calculate the first 8 iterations of the Bisection method on $f(x) = e^{-x}(3.2 \sin(x) - 0.5\cos(x))$ with interval [3, 4].

4. Calculate the first 8 iterations of the Bisection method on $f(x) = x^2 - 3$ with interval [1, 2].

Or

Find the approximate value of square root of 3 using Bisection method . (Do 8 iterations with interval [1,2]).

5. Find the approximate value of square root of 5 using Bisection method correct to two decimal places.