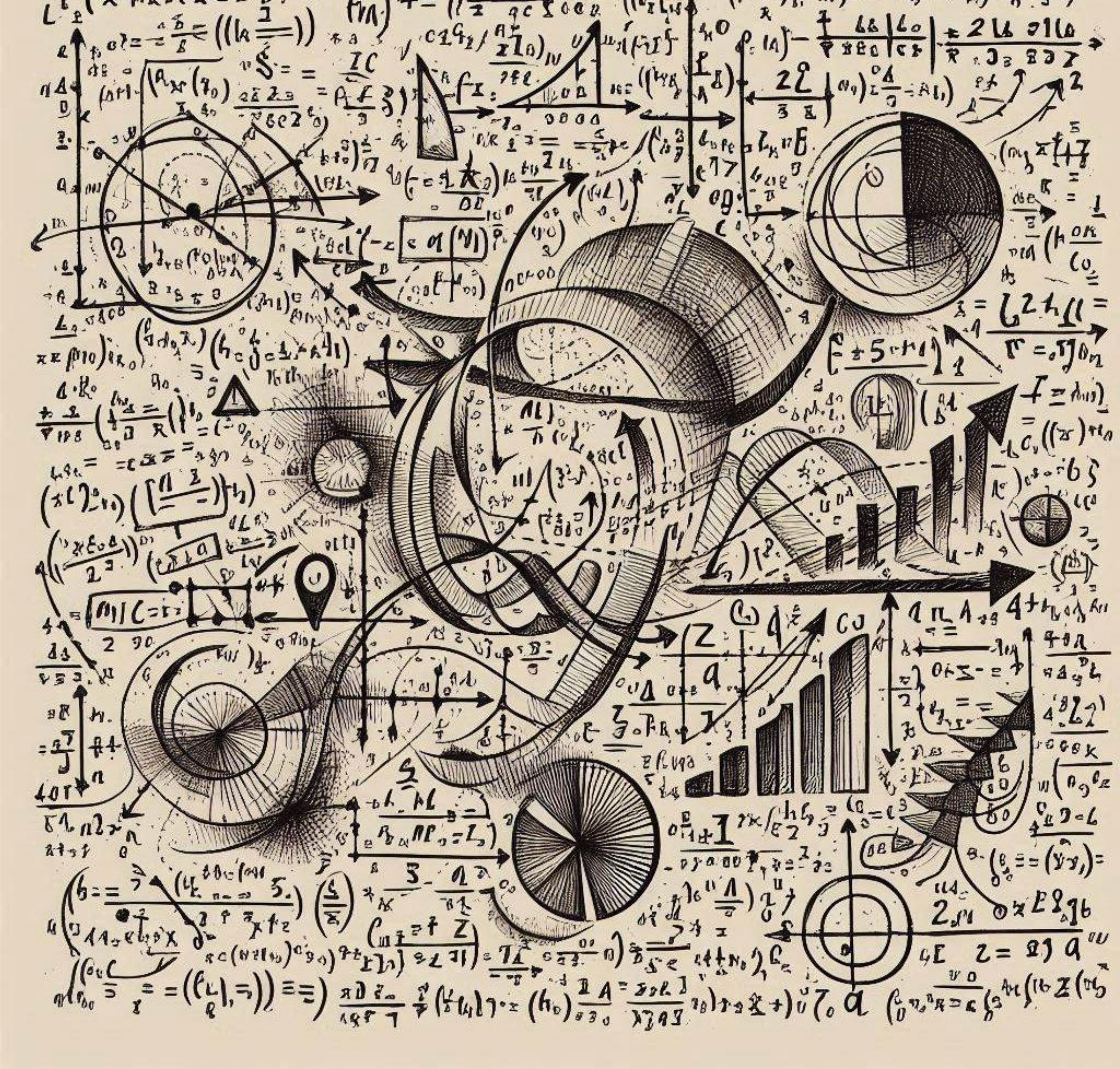
PH 3120 – Computational Physics Laboratory I

Root Finding



Dr. E. M. D. Siriwardane

Department of Physics

University of Colombo

Intermediate Value Theorem

- The Intermediate Value Theorem (IVT) is a fundamental result in calculus that ensures the existence of a root within a continuous interval under certain conditions.
- It is often used in root-finding methods like the bisection method.

Statement of the Intermediate Value Theorem

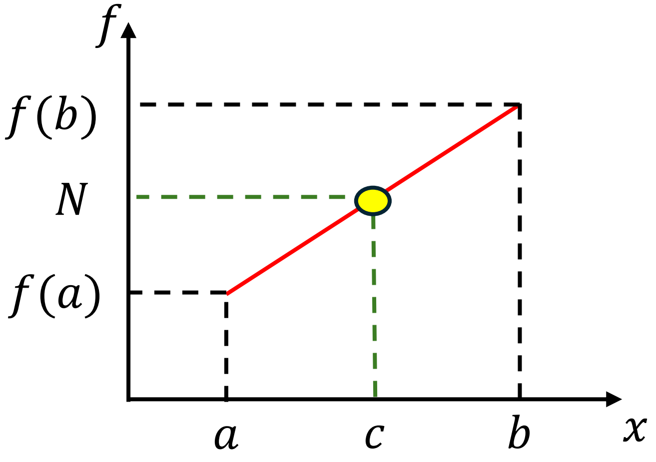
❖ If f is a continuous function on a closed interval $[a, b]$, and N is any number between $f(a)$ and $f(b)$ (inclusive), then there exists at least one number c in the interval (a, b) such that $f(c) = N$.

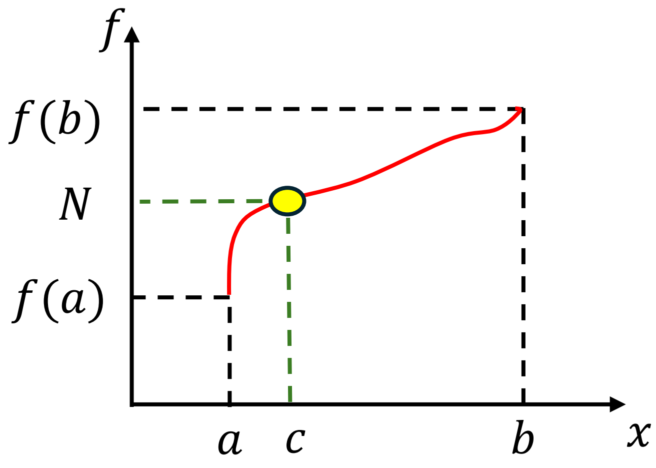
In mathematical notation:

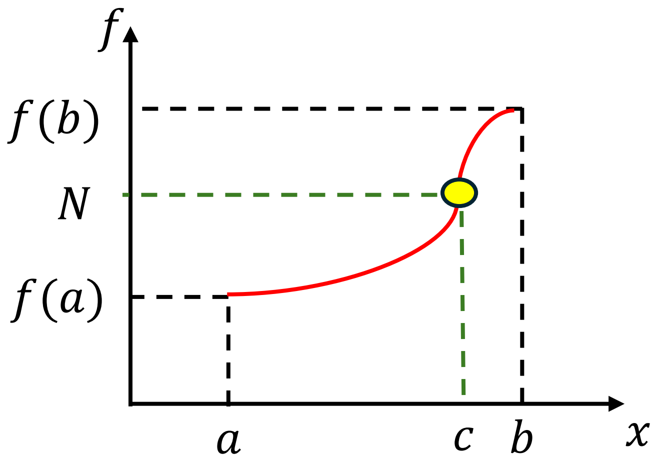
❖ If f is continuous on $[a, b]$ and $f(a) \neq f(b)$, then for any N between $f(a)$ and $f(b)$, there exists $c \in (a, b)$ such that $f(c) = N$.

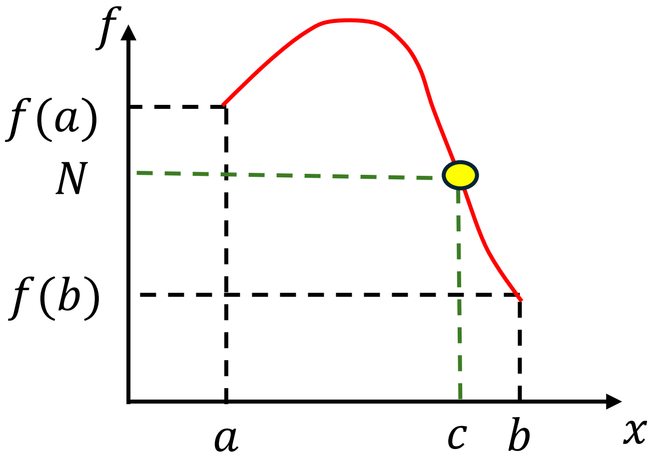
Intermediate Value Theorem

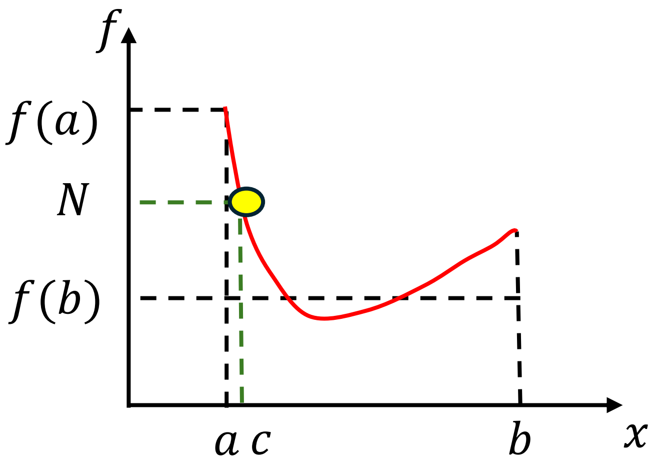
❖ If f is continuous on $[a, b]$ and $f(a) \neq f(b)$, then for any N between $f(a)$ and $f(b)$, there exists $c \in (a, b)$ such that $f(c) = N$.











Intermediate Value Theorem

Example

Consider the function $f(x) = x^3 - x$ on the interval $[-2,2]$. Show that there is some c in $[-2,2]$ such that

$f(c) = 0.$

Solution

Checking the end points

$$f(-2) = (-2)^3 - (-2) = -6$$

$$f(2) = (2)^3 - (2) = 6$$

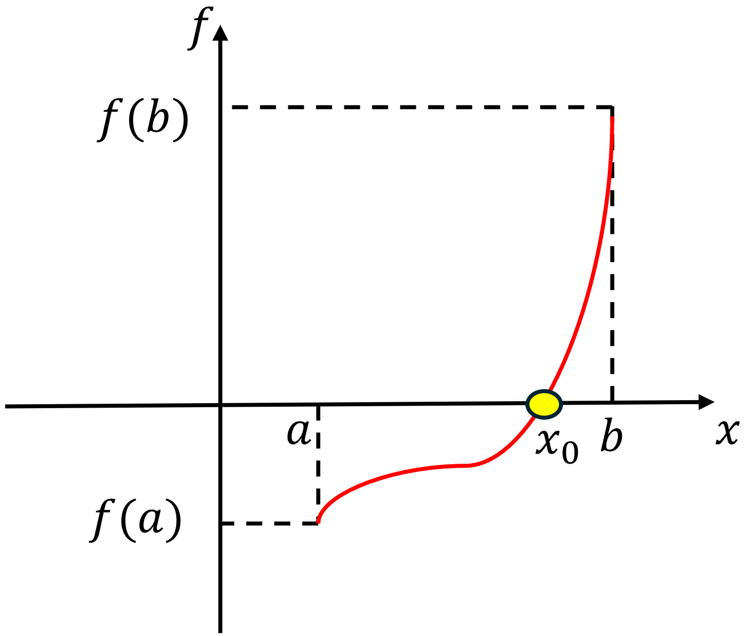
Zero is between $f(-2)$ and $f(2)$. Therefore, there is a x value within the intervale $[-2,2]$ such that $f(x) = 0$

$$f(-1) = (-1)^3 - (-1) = -1 + 1 = 0$$

Bisection Method

The IVT ensures that if $f(a) \cdot f(b) < 0$, then there is at least one root in the interval (a, b).

The bisection method finds the root by repeatedly applying the IVT to subintervals.



Step 1

Choose two points a and b such that $f(a) \cdot f(b) < 0$.

This ensures that there is at least one root in the interval $[a, b]$ by the Intermediate Value Theorem.

Bisection Method

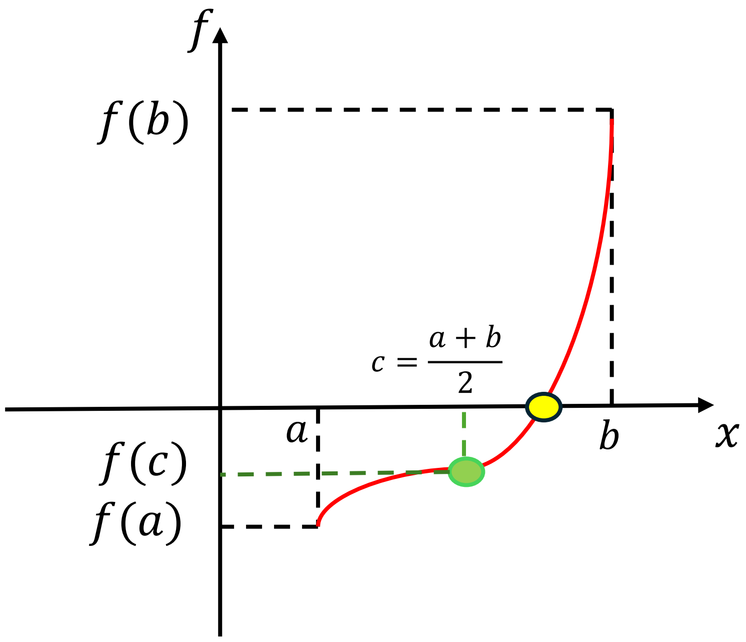
Step 2

Calculate the midpoint $c = \frac{a+b}{2}$

Step 3

Evaluate function at the midpoint

Calculate $f(c)$

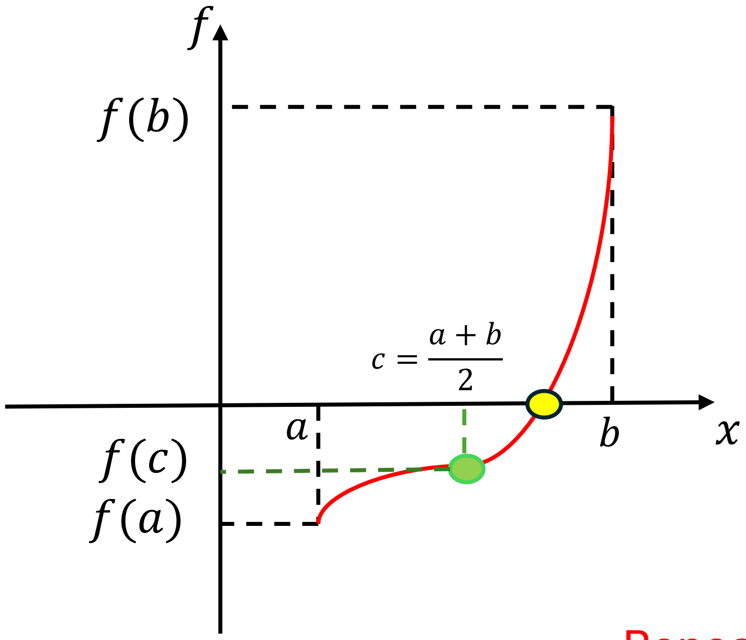


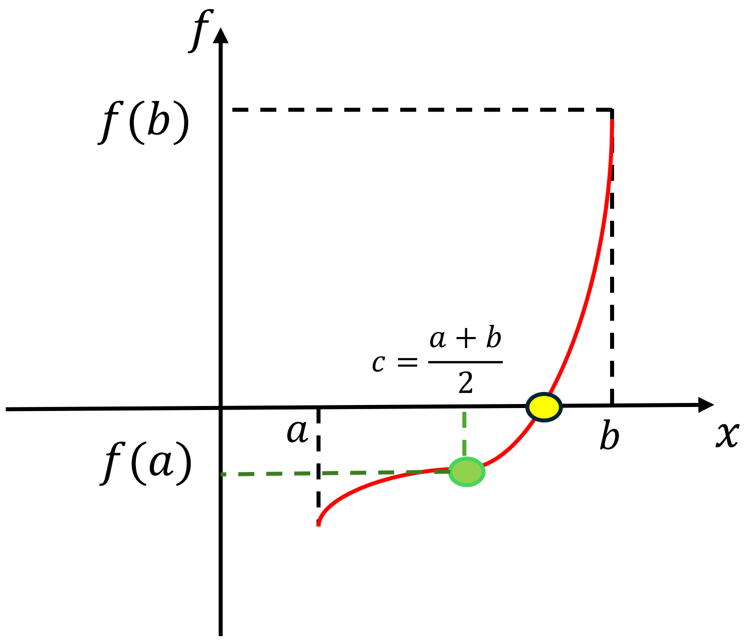
Bisection Method

Step 4

Check for Root:

- If $f(c) = 0$ or $|\, b - a \,|$ is sufficiently small (below a predefined tolerance ϵ), then c is the root.
- If $f(a) \cdot f(c) < 0$, set $b = c$ (the root is in the left subinterval).
- If $f(b) \cdot f(c) < 0$, set $a = c$ (the root is in the right subinterval).





Repeat steps 2-4 until convergence.

Bisection Method

Algorithm

```
function bisection(f, a, b, tol)
    if f(a) * f(b) >= 0
        error "The function must have opposite signs at a and b."
    end if

    while (b - a) / 2 > tol
        c = (a + b) / 2
        if f(c) == 0
            return c
        end if

        if f(a) * f(c) < 0
            b = c
        else
            a = c
        end if
    end while

    return (a + b) / 2
end function
```

Bisection Method

Example

Consider the function $f(x) = x^3 - x + 1$ on the interval $[-2,2]$. Show that there is some c in $[-2,2]$ such that $f(c) = 0.$

Solution

Checking the end points

$$f(-2) = (-2)^3 - (-2) + 1 = -5$$

$$f(2) = (2)^3 - (2) + 1 \ = 7$$

$$f(-2) \times f(2) = -35 < 0$$

Therefore, there is a root in [-2,2]

Bisection Method

$f(x) = x^3 - x + 1$

1

$$c = \frac{a+b}{2} = \frac{-2+2}{2} = 0$$

$$f(c) = f(0) = 1$$

This gives us,

$$f(0) \times f(-2) = -5 < 0$$

Therefore, $b = c = 0$

2

$$c = \frac{a+b}{2} = \frac{-2+0}{2} = -1 \qquad a = -2, \qquad b = 0$$

$$f(c) = f(-1) = 1$$

This gives us,

$$f(1) \times f(-2) = -5 < 0$$

Therefore, $b = c = -1$

3

$$c = \frac{a+b}{2} = \frac{-2+(-1)}{2} = -1.5 \qquad a = -2, \qquad b = -1$$

$$f(c) = f(-1.5) = -0.875$$

This gives us,

$$f(-1.5) \times f(-1) = -0.875 < 0$$

Therefore, $a = c = -1.5$

4

$$c = \frac{a+b}{2} = \frac{-1.5+(-1)}{2} = -1.25 \qquad a = -1.5, \qquad b = -1$$

$$f(c) = f(-1.25) = 0.297$$

This gives us,

$$f(-1.25) \times f(-1.5) < 0$$

Therefore, $a = c = -1.25$