

Computational Physics



Lecture-12

M. Reza Mozaffari

Physics Group, University of Qom

Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root

Numerical Finding Root

- **Bisection Method**

Step 1: Calculate the **midpoint** of the interval

$$c_n = \frac{a_n + b_n}{2}$$

Step 2: Check if it has **converged** to a root within acceptable precision

$$|f(c_n)| < \epsilon, \quad \epsilon \ll 1$$

Step 3: New interval,

$$f(a_n)f(c_n) > 0$$

$$[a_{n+1}, b_{n+1}] = [c_n, b_n]$$

$$f(a_n)f(c_n) < 0$$

$$[a_{n+1}, b_{n+1}] = [a_n, c_n]$$

Step 4: Return to **Step 1**

Numerical Finding Root

- Newton-Raphson

Step 1: The equation of the tangent line,

$$L_n : y = f(x_n) + f'(x_n)(x - x_n)$$

Step 2: The tangent line intersects the x-axis and new point,

$$y(x_{n+1}) = 0$$
$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Step 3: Check if it has **converged** to a root within acceptable precision

$$|x_{n+1} - x_n| < \epsilon, \quad \epsilon \ll 1$$

Step 4: Return to **Step 1**

Numerical Finding Root

- Secant

Step 1: The equation of the tangent line,

$$L_n : y = f(x_n) + m(x - x_n)$$

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

Step 2: The tangent line intersects the x-axis and new point,

$$y(x_{n+1}) = 0$$

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

Step 3: Check if it has **converged** to a root within acceptable precision

$$|x_{n+1} - x_n| < \epsilon, \quad \epsilon \ll 1$$

Step 4: Return to **Step 1**

Numerical Finding Root

- False Position Method

Step 1: Calculate the midpoint of the interval

$$y(c_n) = 0$$

$$c_n = a_n - f(a_n) \left(\frac{b_n - a_n}{f(b_n) - f(a_n)} \right)$$

Step 2: Check if it has converged to a root within acceptable precision

$$|f(c_n)| < \epsilon, \quad \epsilon \ll 1$$

Step 3: New interval,

$$f(a_n)f(c_n) > 0$$

$$[a_{n+1}, b_{n+1}] = [c_n, b_n]$$

$$f(a_n)f(c_n) < 0$$

$$[a_{n+1}, b_{n+1}] = [a_n, c_n]$$

Step 4: Return to Step 1