Computational Physics

Lecture-10

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Contents

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

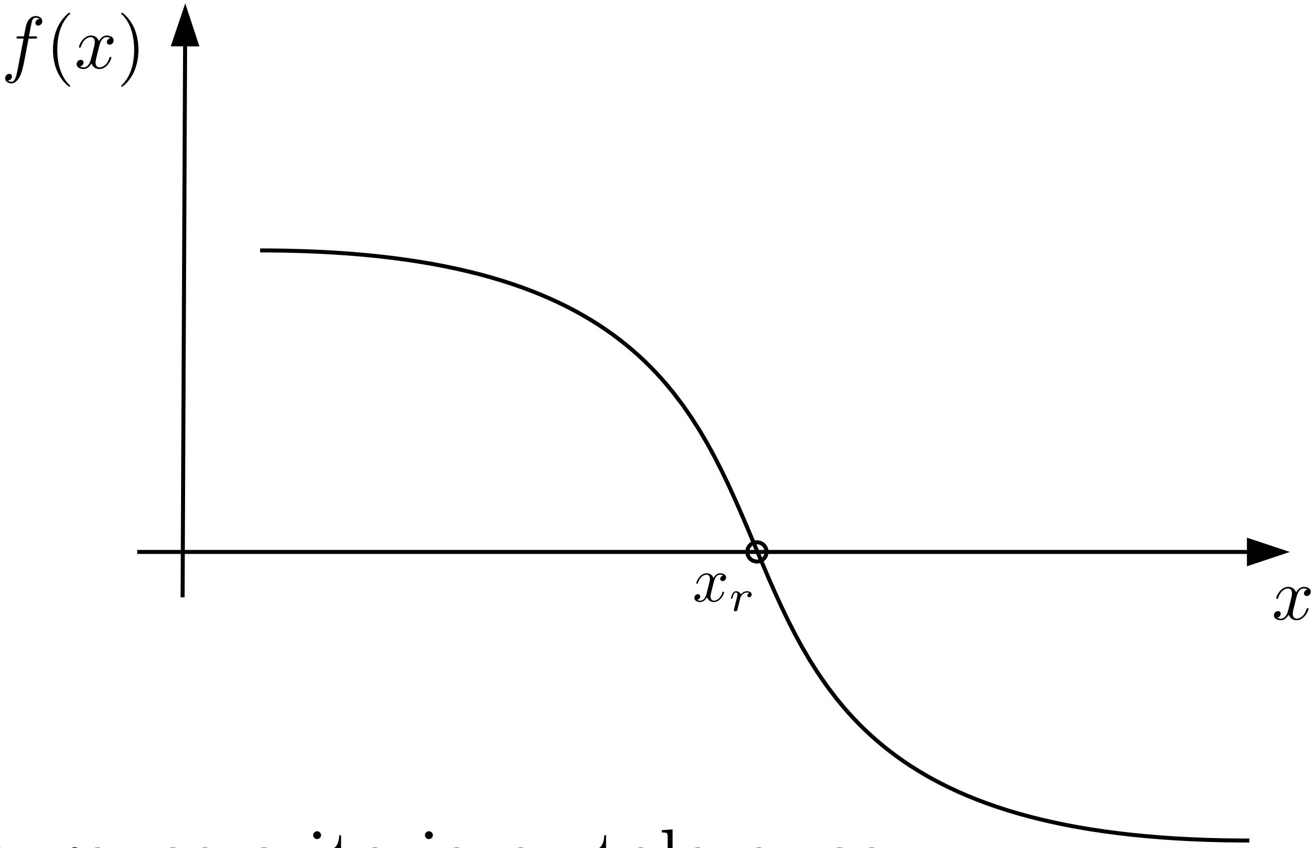
Numerical Finding Root

Analytically

$$f(x_r) = 0$$

Numerically

$$\lim_{x \to x_r} f(x) \to 0$$



$$|f(x_r)| < \epsilon, \quad \epsilon \text{ is a convergence criteria or tolerance.}$$

$$\epsilon \ll 1$$

Numerical Finding Root

- **Bisection Method (Bracketed Method)**

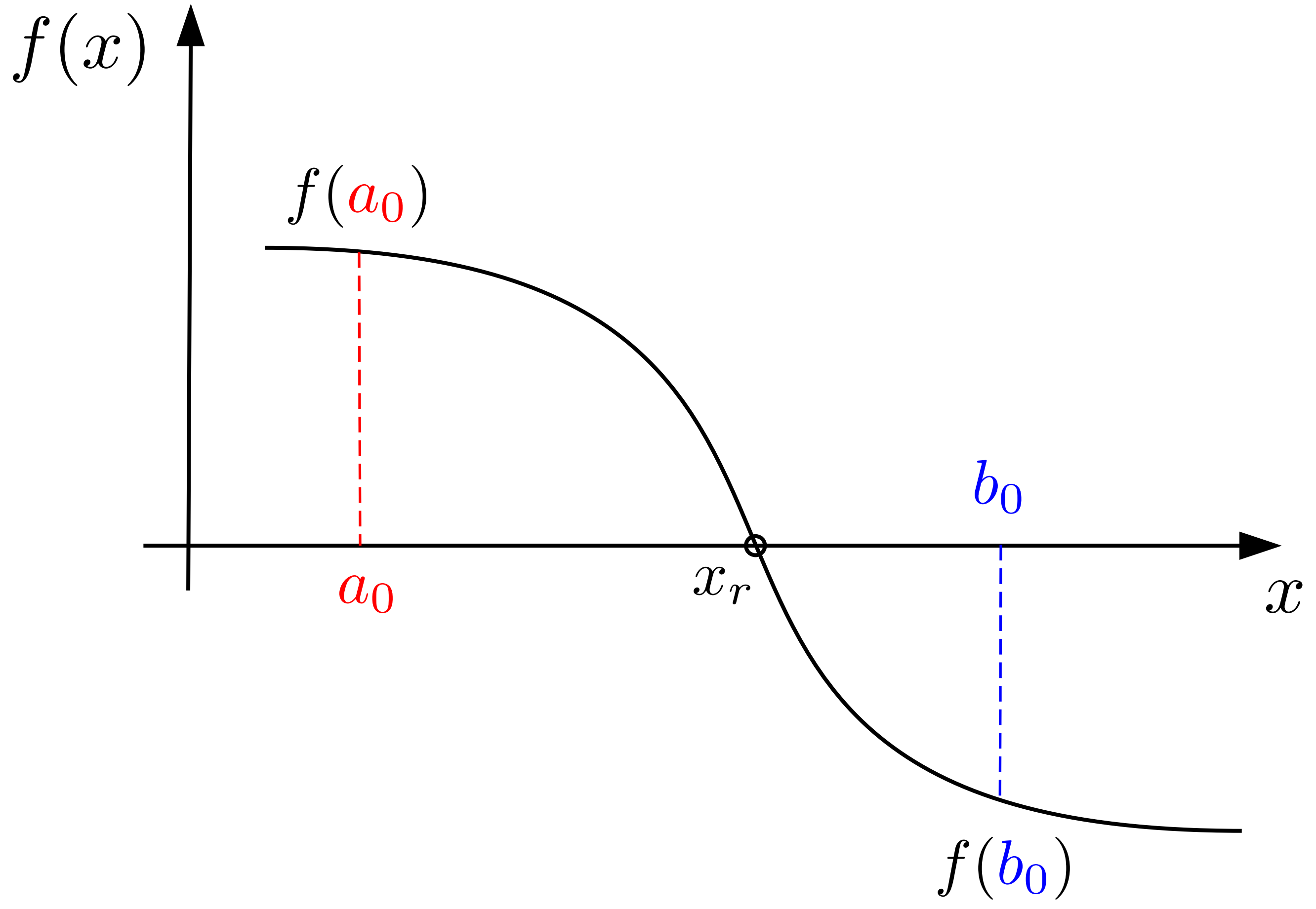
Step 0:

Choose an appropriate interval

$$x_r \in [a_0, b_0]$$

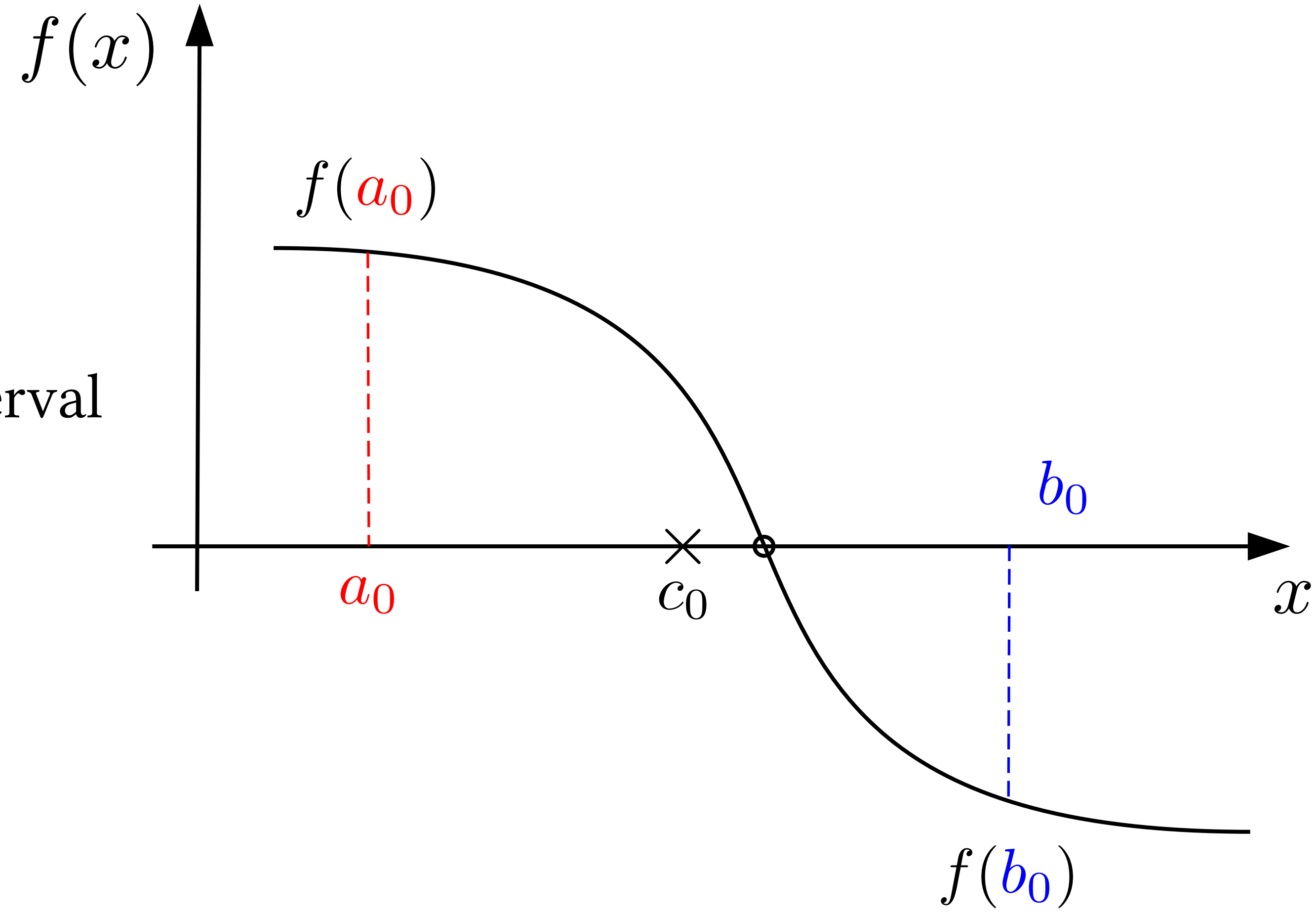
Such that

$$f(a_0)f(b_0) < 0$$



Numerical Finding Root

- **Bisection Method**



Step 1:

Calculate the **midpoint** of the interval

$$c_0 = \frac{a_0 + b_0}{2}$$

Numerical Finding Root

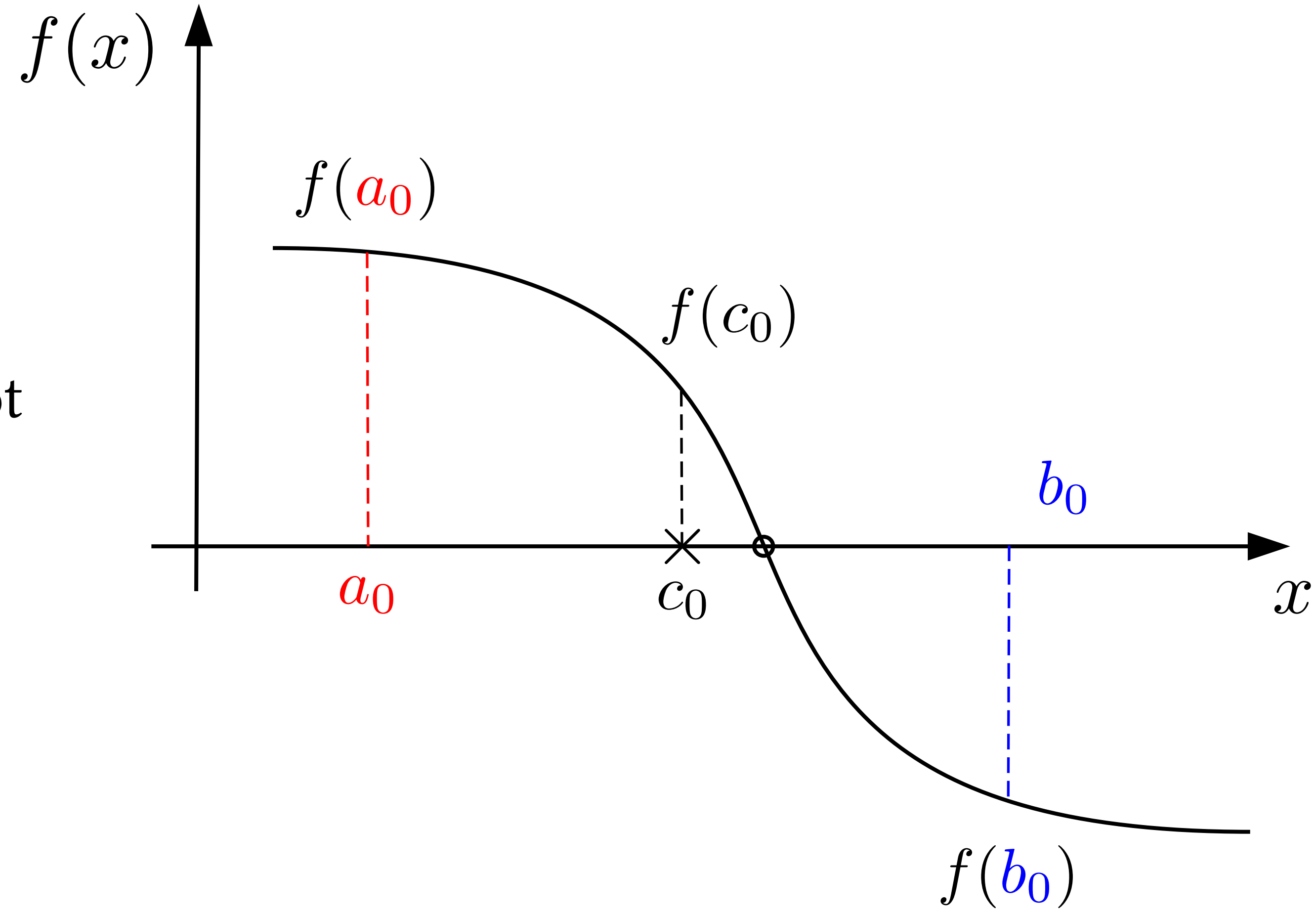
- **Bisection Method**

Step 2:

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

$$|f(c_0)| < \epsilon$$

$$\epsilon \ll 1$$



Numerical Finding Root

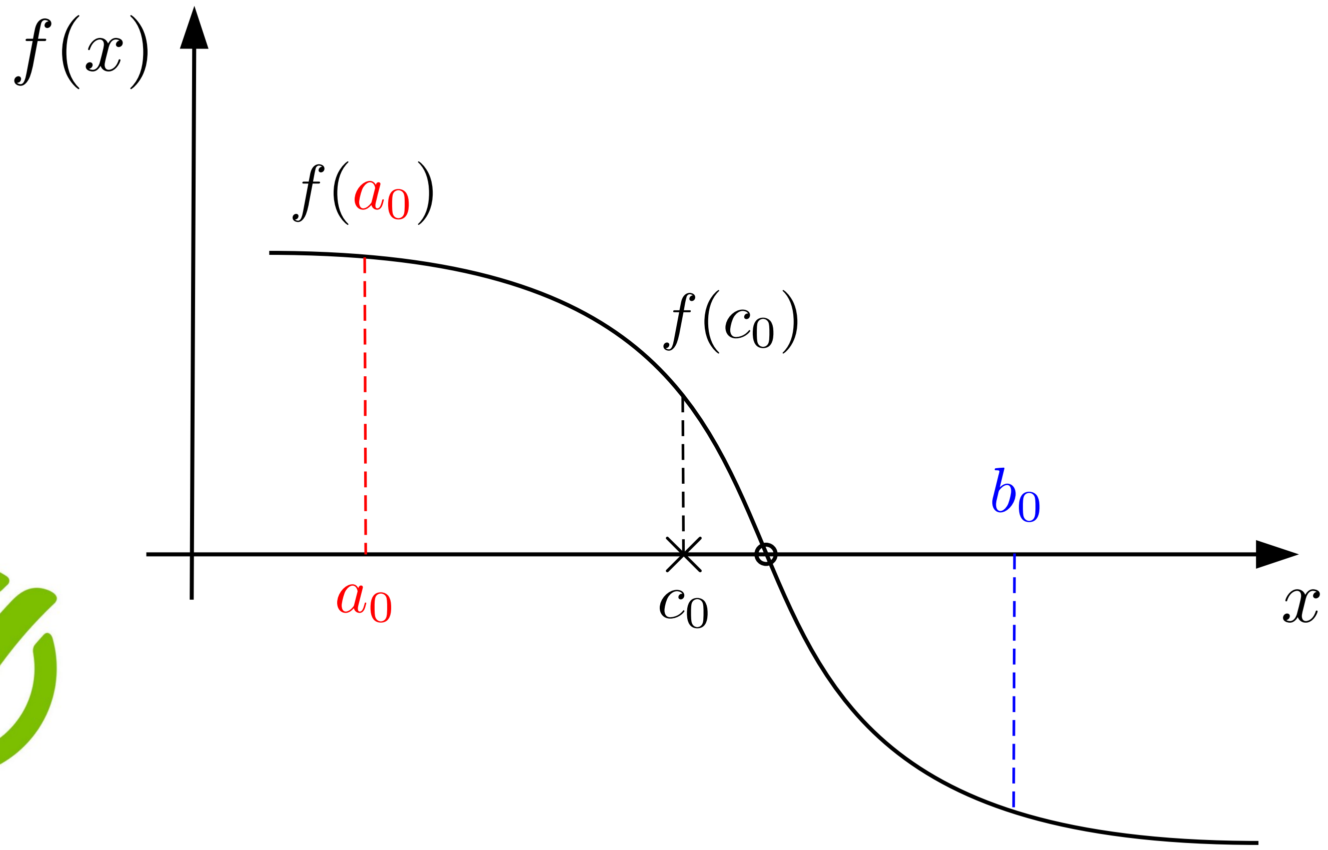
- **Bisection Method**

Step 3:

New interval,

$$f(a_0)f(c_0) > 0$$

$$f(a_0)f(c_0) < 0$$



Numerical Finding Root

- **Bisection Method**

Step 3:

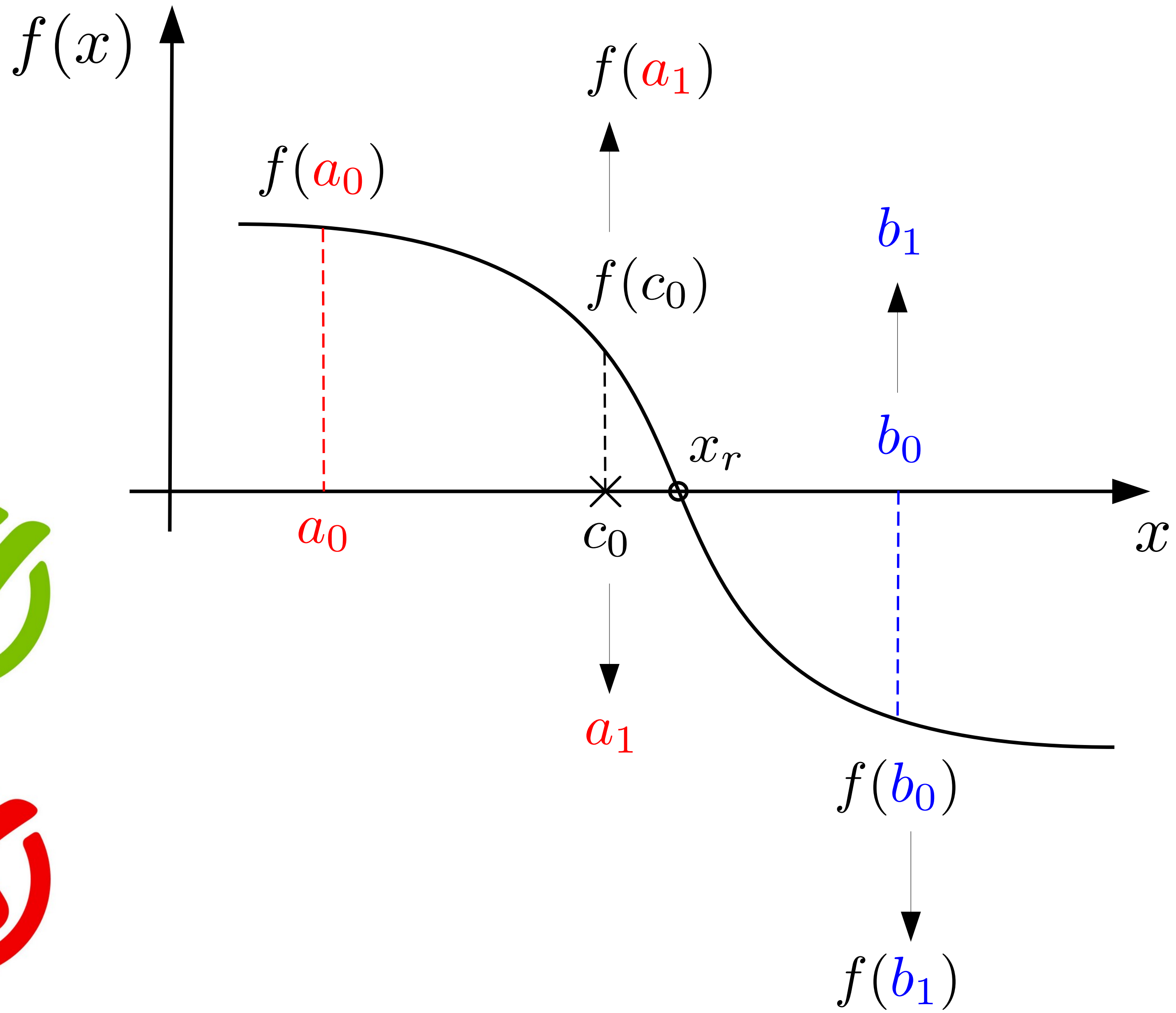
New interval,

$$f(a_0)f(c_0) > 0$$

$$[a_1, b_1] = [c_0, b_0]$$

$$f(a_0)f(c_0) < 0$$

$$[a_1, b_1] = [a_0, c_0]$$

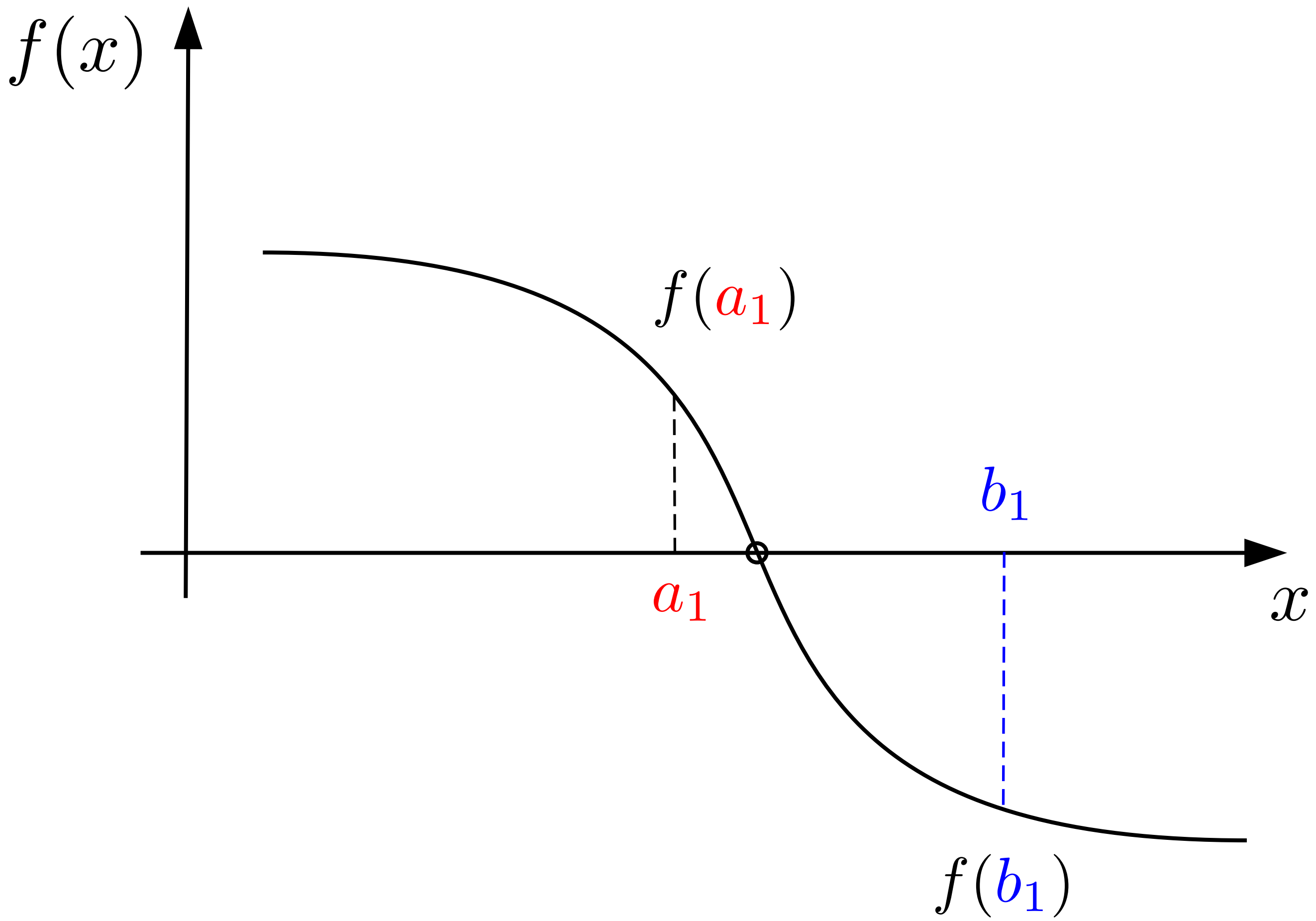


Numerical Finding Root

- **Bisection Method**

Step 4:

Return to Step 1



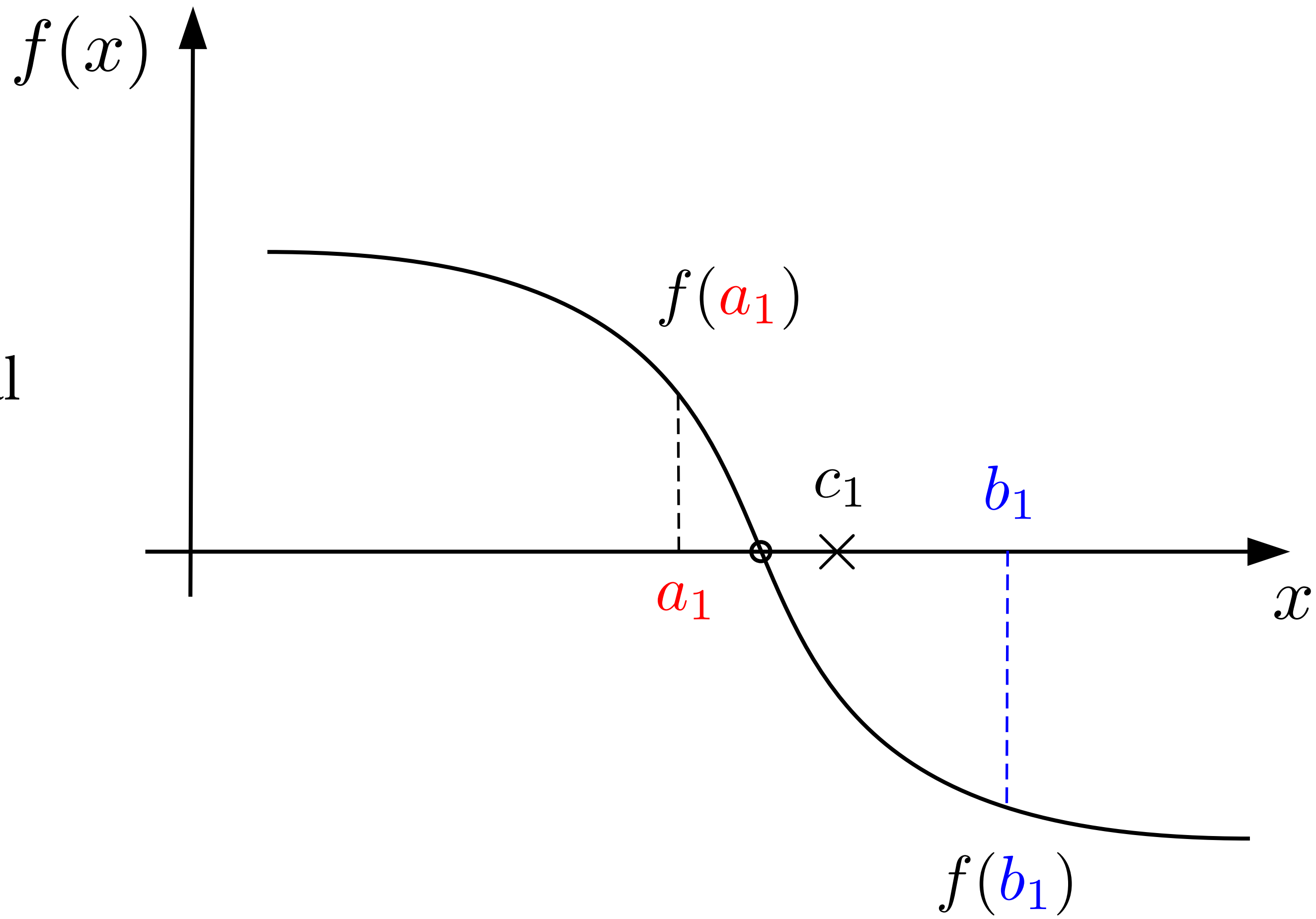
Numerical Finding Root

- **Bisection Method**

Step 1:

Calculate the **midpoint** of the interval

$$c_1 = \frac{a_1 + b_1}{2}$$



Numerical Finding Root

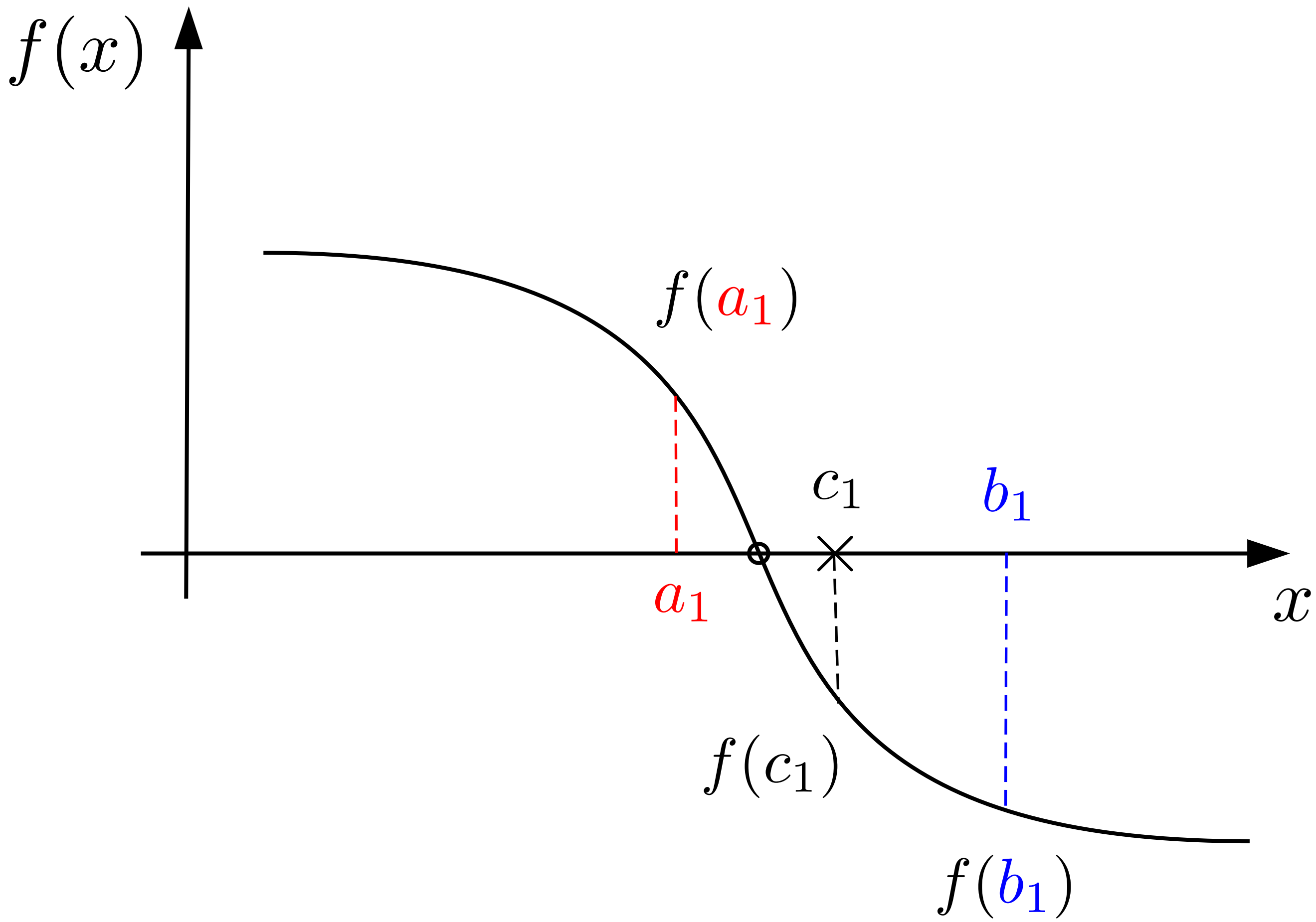
- **Bisection Method**

Step 2:

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

$$|f(c_1)| < \epsilon$$

$$\epsilon \ll 1$$



Numerical Finding Root

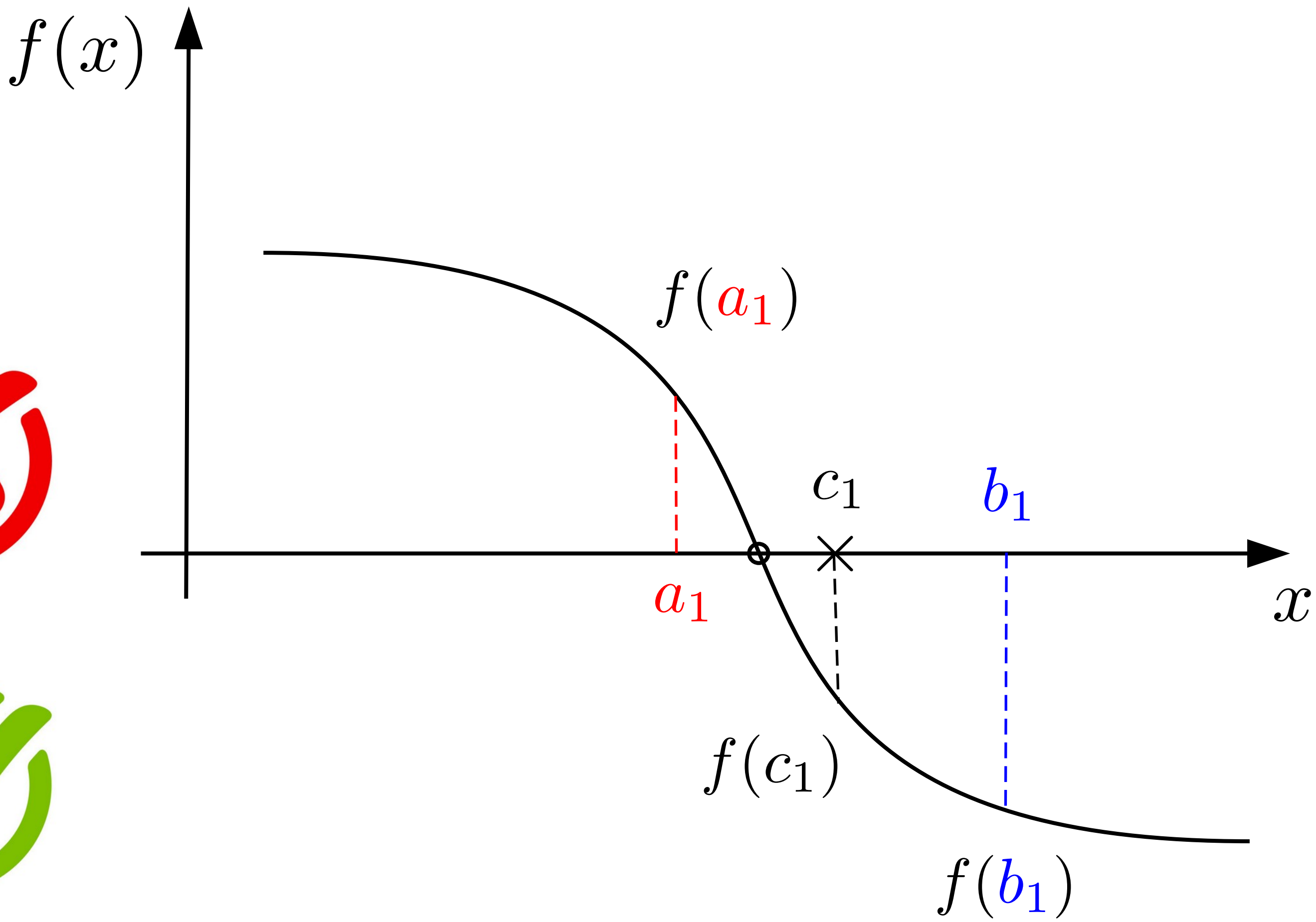
- **Bisection Method**

Step 3:

New interval,

$$f(a_1)f(c_1) > 0$$

$$f(a_1)f(c_1) < 0$$



Numerical Finding Root

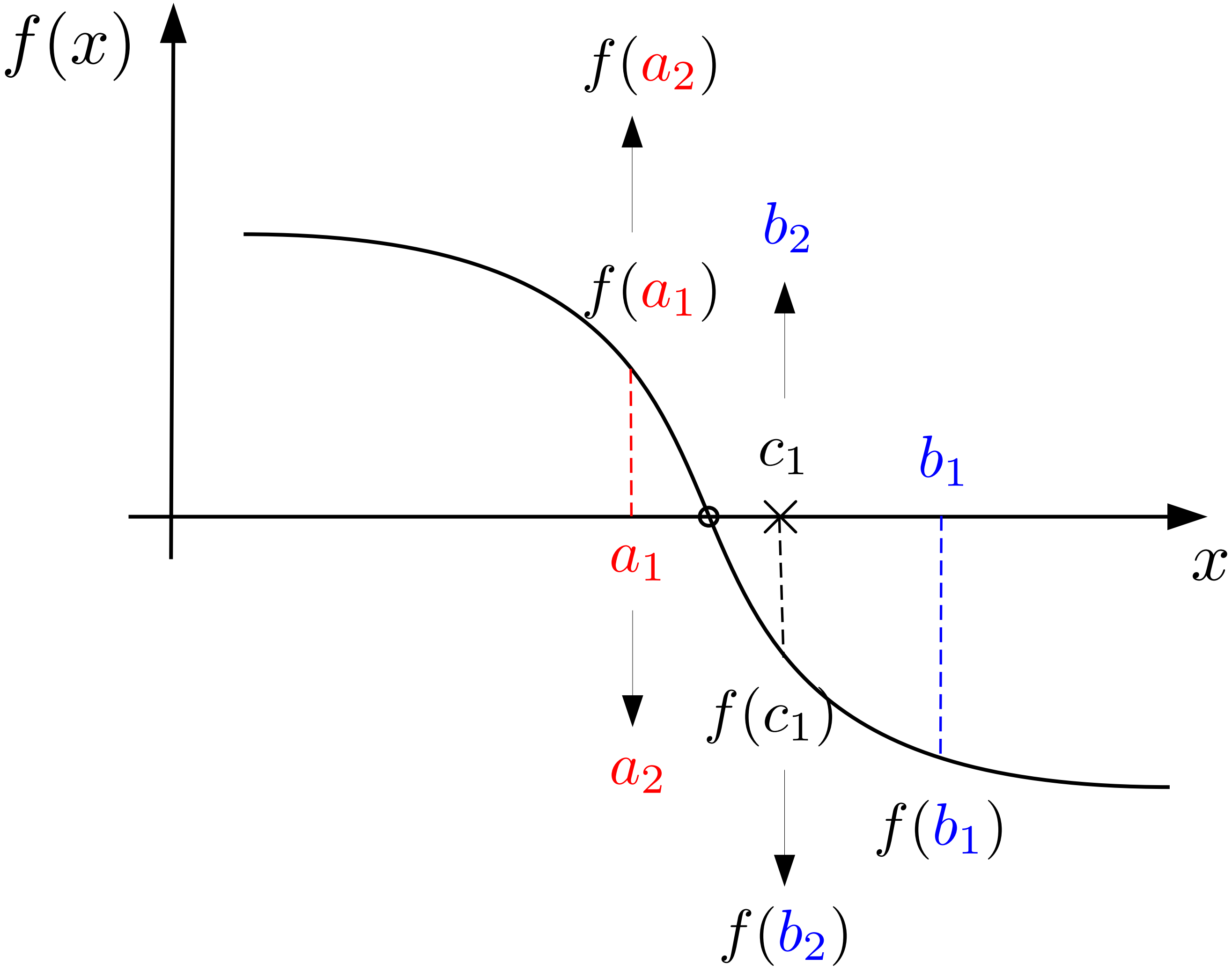
- **Bisection Method**

Step 3:

New interval,

$$f(a_1)f(c_1) > 0$$
$$[a_2, b_2] = [c_1, b_1]$$

$$f(a_1)f(c_1) < 0$$
$$[a_2, b_2] = [a_1, c_1]$$

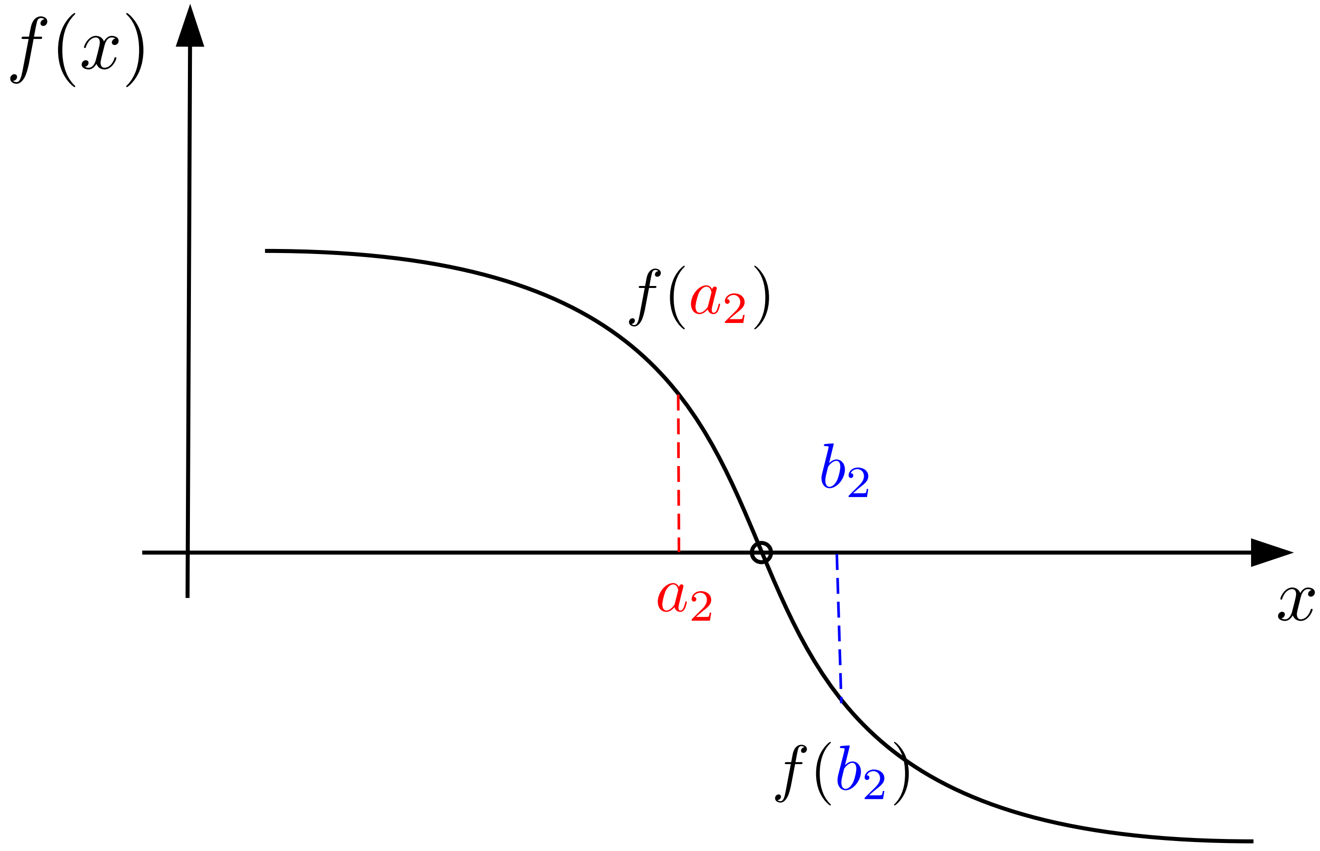


Numerical Finding Root

- **Bisection Method**

Step 4:

Return to Step 1



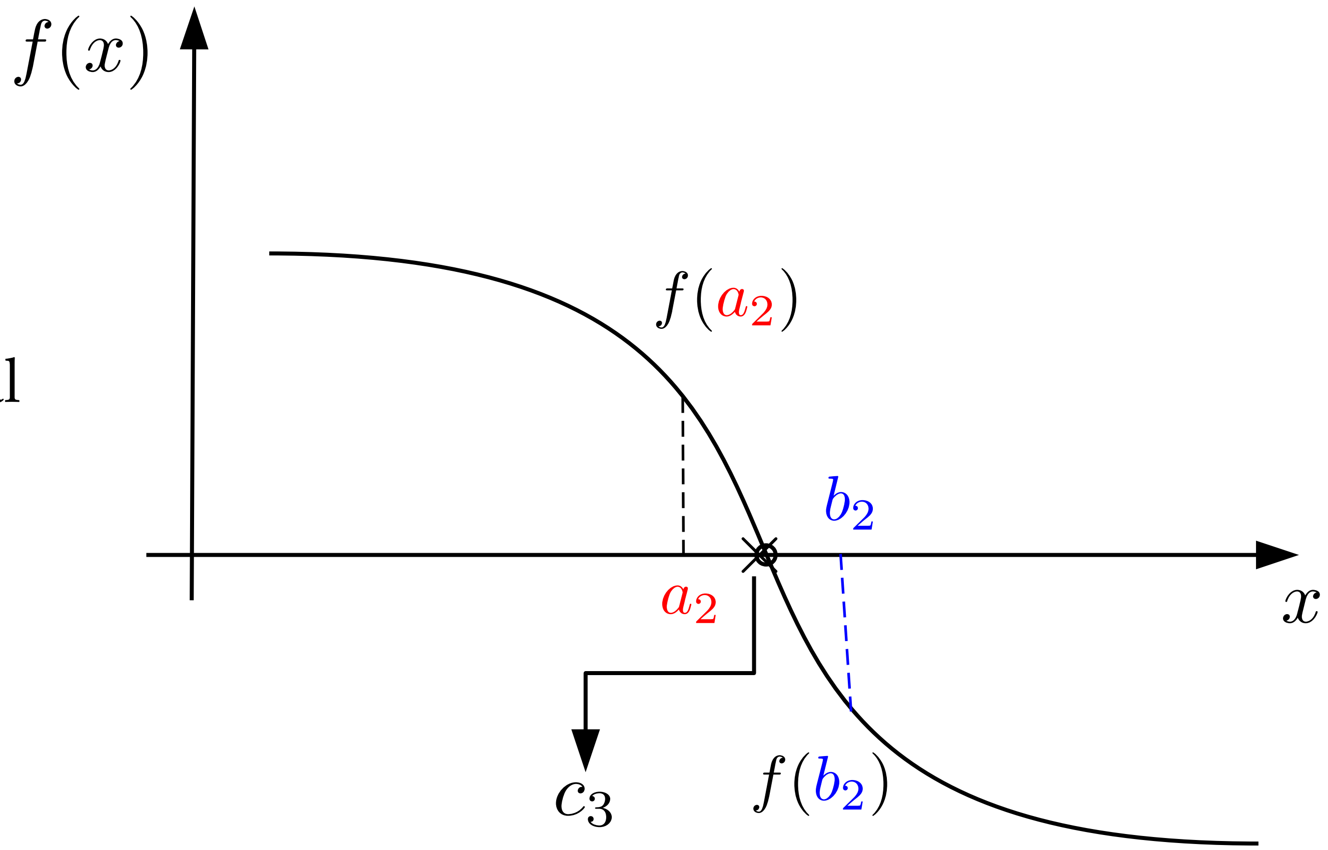
Numerical Finding Root

- **Bisection Method**

Step 1:

Calculate the **midpoint** of the interval

$$c_3 = \frac{a_2 + b_2}{2}$$



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**,

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

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

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

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

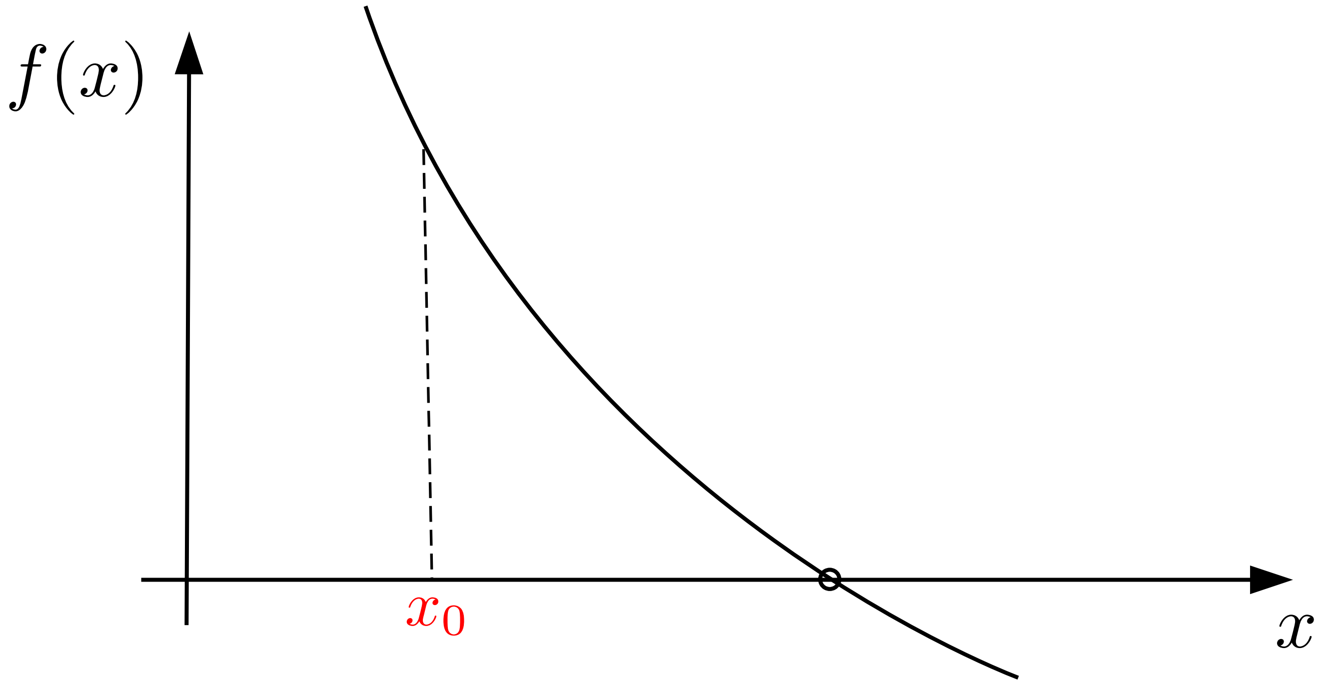
Step 4: Return to **Step 1**

Numerical Finding Root

Nature and Nature's laws lay hid in night:
God said, Let Newton be! And all was light.
Alexander Pope, 1727

- **Newton-Raphson**

Step 0: An initial guess

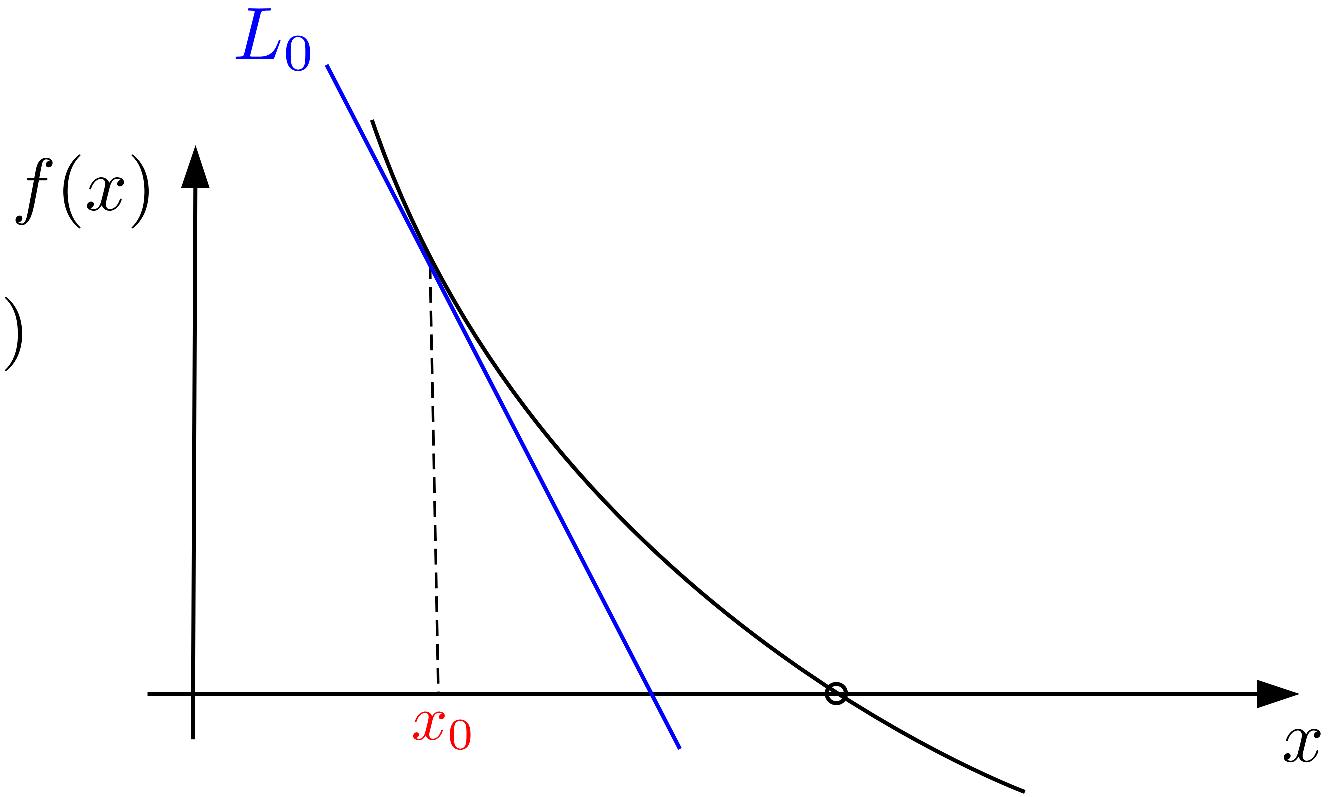


Numerical Finding Root

- **Newton-Raphson**

Step 1: The equation of the tangent line,

$$L_0 : \; y = f(x_0) + f'(x_0)(x - x_0)$$



Numerical Finding Root

- **Newton-Raphson**

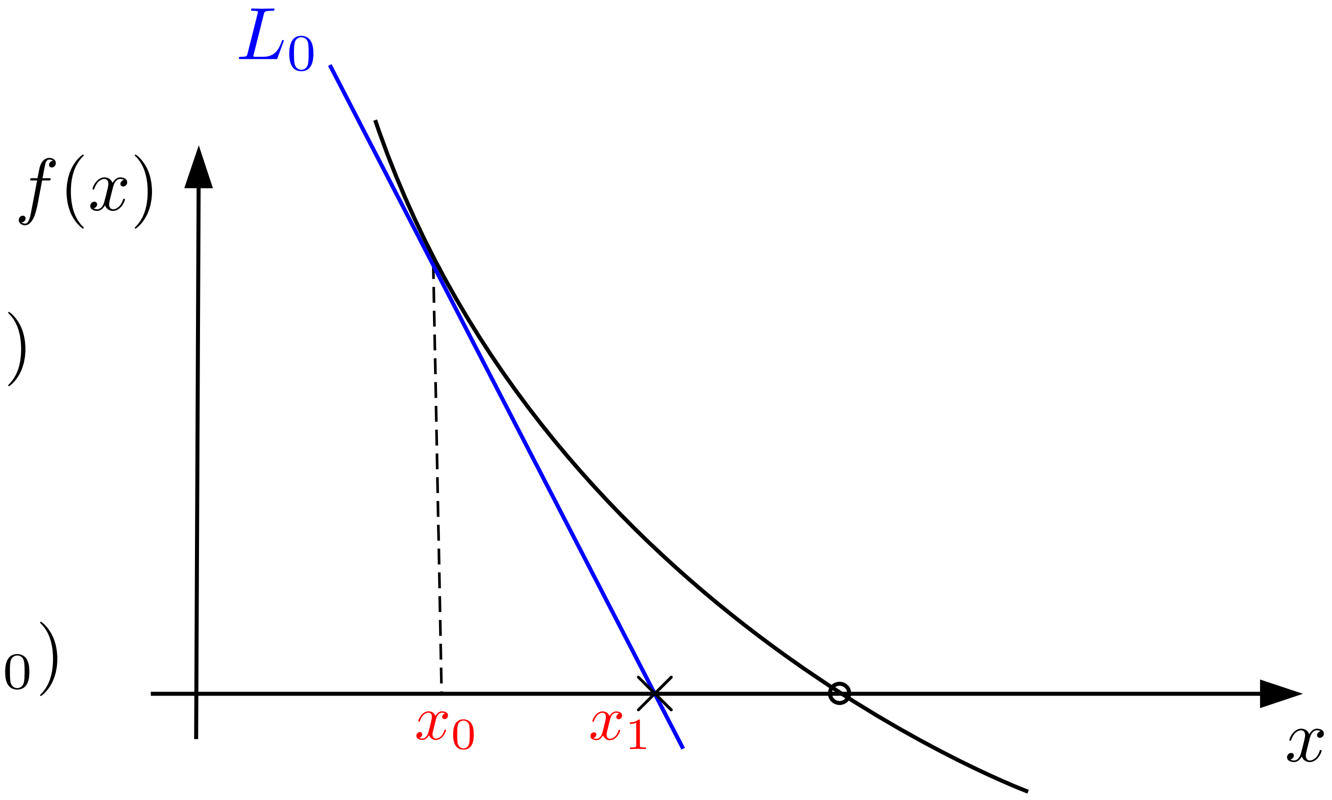
Step 2: The tangent line intersects the x-axis and new point,

$$L_0 : \; y = f(x_0) + f'(x_0)(x - x_0)$$

$$y(x_1) = 0$$

$$0 = f(x_0) + f'(x_0)(x_1 - x_0)$$

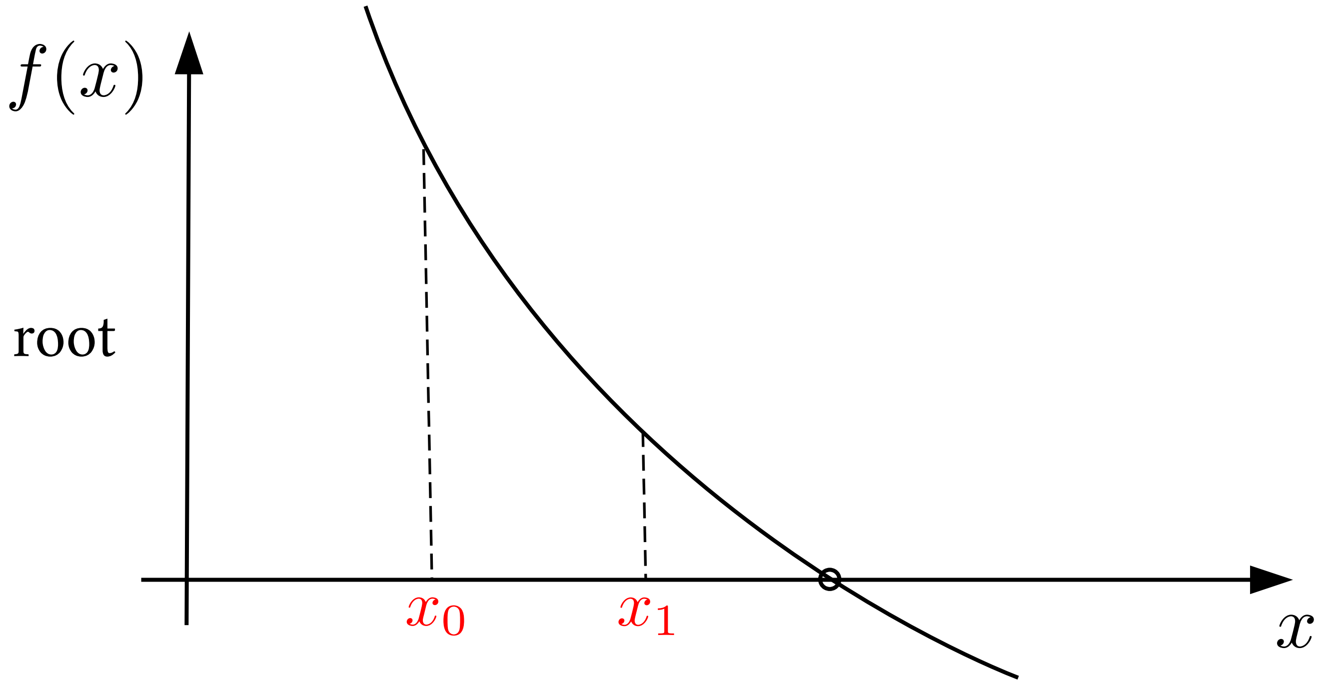
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$



Numerical Finding Root

- **Newton-Raphson**

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$



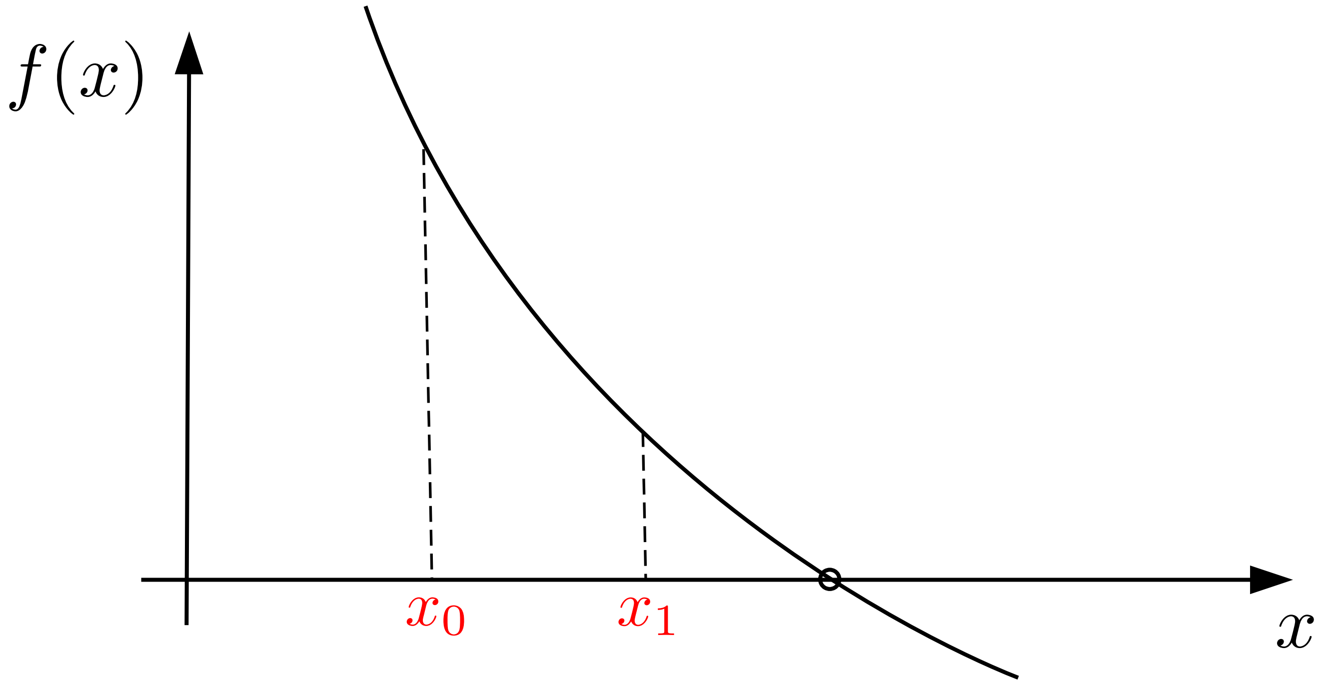
Step 3: Check if it has **converged** to a root within acceptable precision

$$|x_1 - x_0| < \epsilon, \quad \epsilon \ll 1$$

Numerical Finding Root

- **Newton-Raphson**

Step 4: Return to **Step 1**.

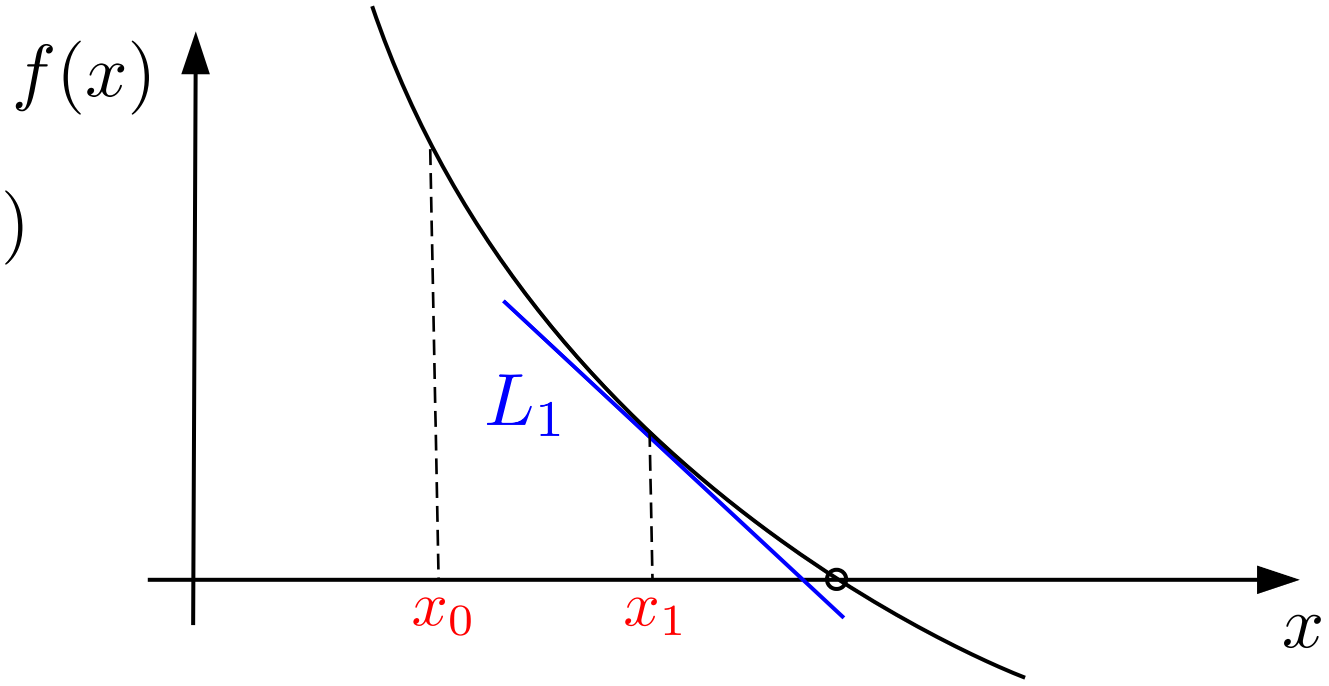


Numerical Finding Root

- **Newton-Raphson**

Step 1: The equation of the tangent line,

$$L_1 : \; y = f(x_1) + f'(x_1)(x - x_1)$$



Numerical Finding Root

- **Newton-Raphson**

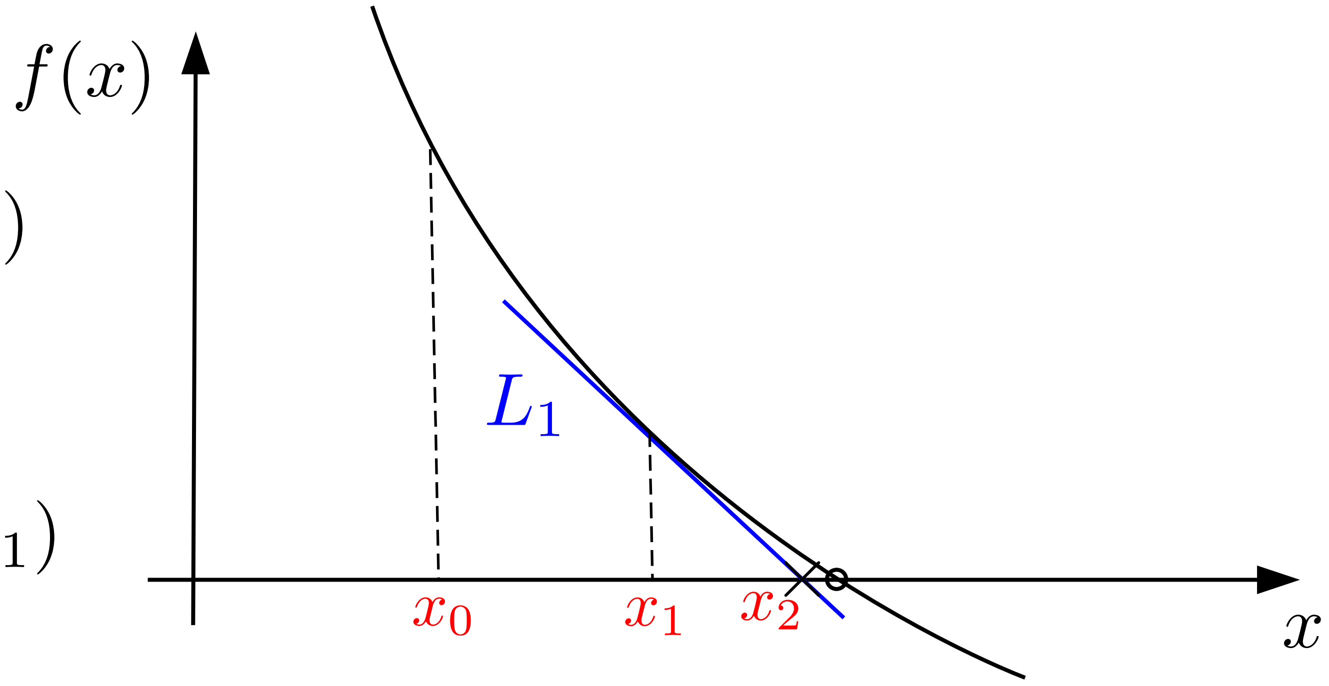
Step 2: The tangent line intersects the x-axis and new point,

$$L_1 : y = f(x_1) + f'(x_1)(x - x_1)$$

$$y(x_2) = 0$$

$$0 = f(x_1) + f'(x_1)(x_2 - x_1)$$

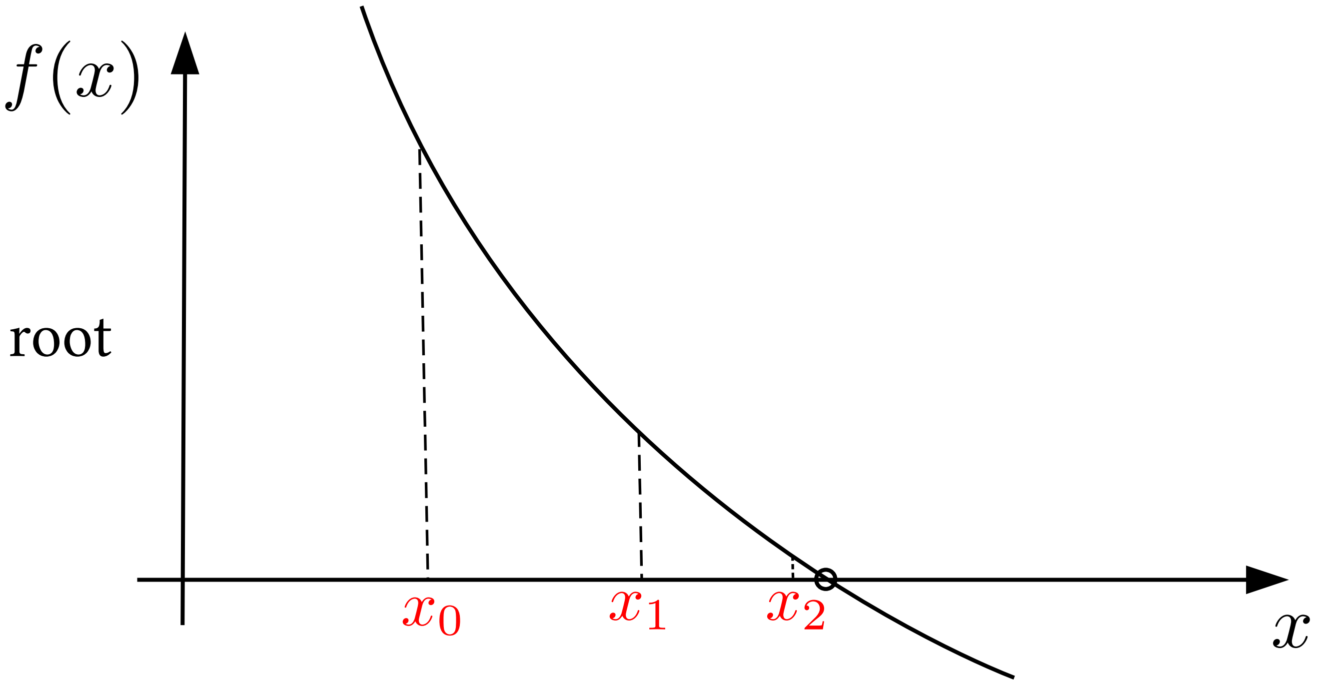
$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$



Numerical Finding Root

- **Newton-Raphson**

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$



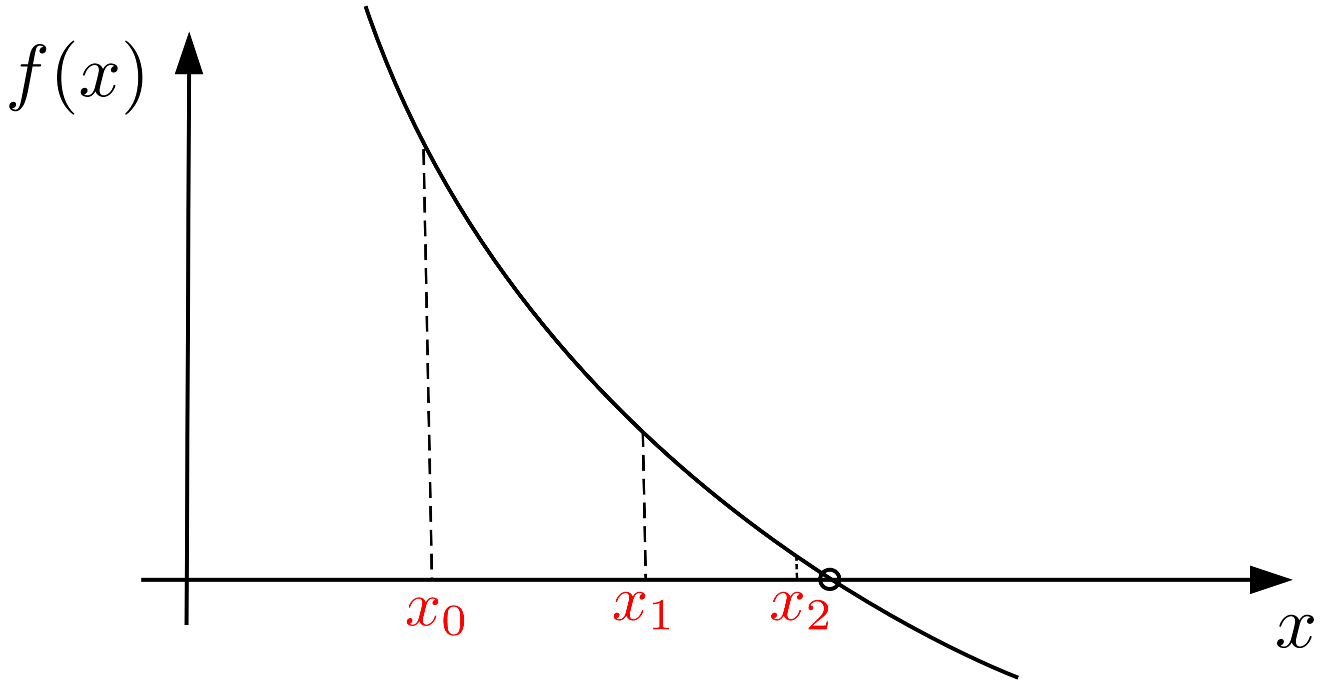
Step 3: Check if it has **converged** to a root within acceptable precision

$$|x_2 - x_1| < \epsilon, \quad \epsilon \ll 1$$

Numerical Finding Root

- **Newton-Raphson**

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**