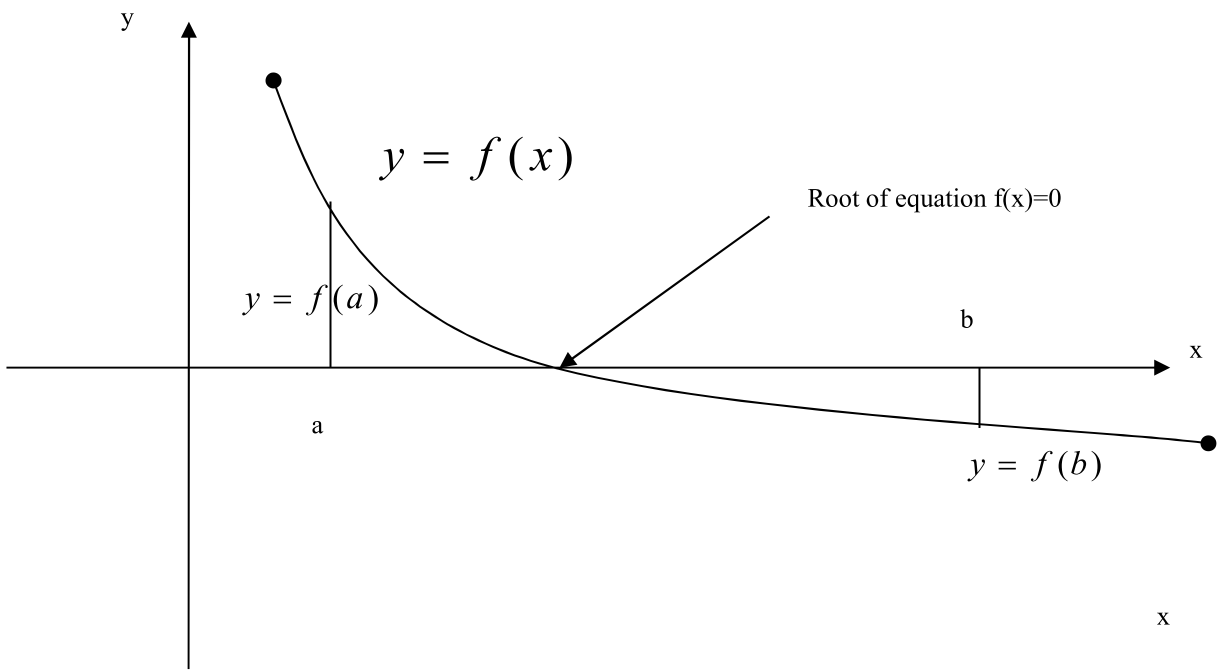
Chapter 1: Computer Solution of Nonlinear Equations

Finding the root of equation f(x)=0, for examples:

(1) Transcendental Equations $f(x) = e^{-x} - \sin(\pi x/2) = 0$

(2) Polynomial equations $f(x) = x^4 - x^3 - 10x^2 - x + 1 = 0$

Graphical method by plotting f(x) against x



Roots of Polynomial Equations

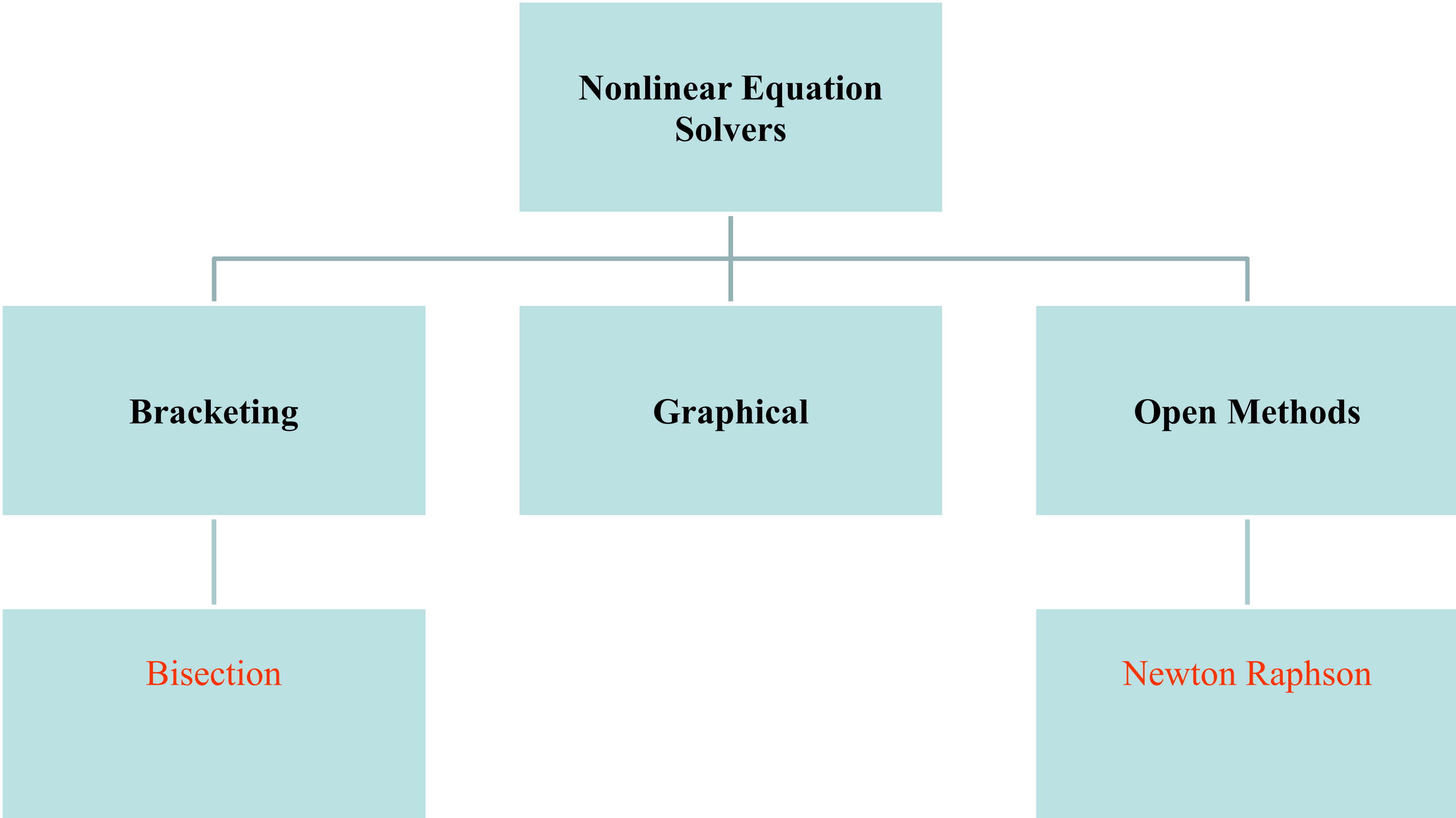
- Why?

$$ax^2 + bx + c = 0 \quad \Rightarrow \quad x = \frac{-b \mp \sqrt{b^2 - 4ac}}{2a}$$

- But

$$ax^5 + bx^4 + cx^3 + dx^2 + ex + f = 0 \quad \Rightarrow x = ?$$

$$\sin x + x = 0 \quad \Rightarrow x = ?$$


Nonlinear Equation Solvers
Bracketing
Graphical
Open Methods
Bisection
Newton Raphson

1.1 Numerical method : Bisection (Bracketing) method

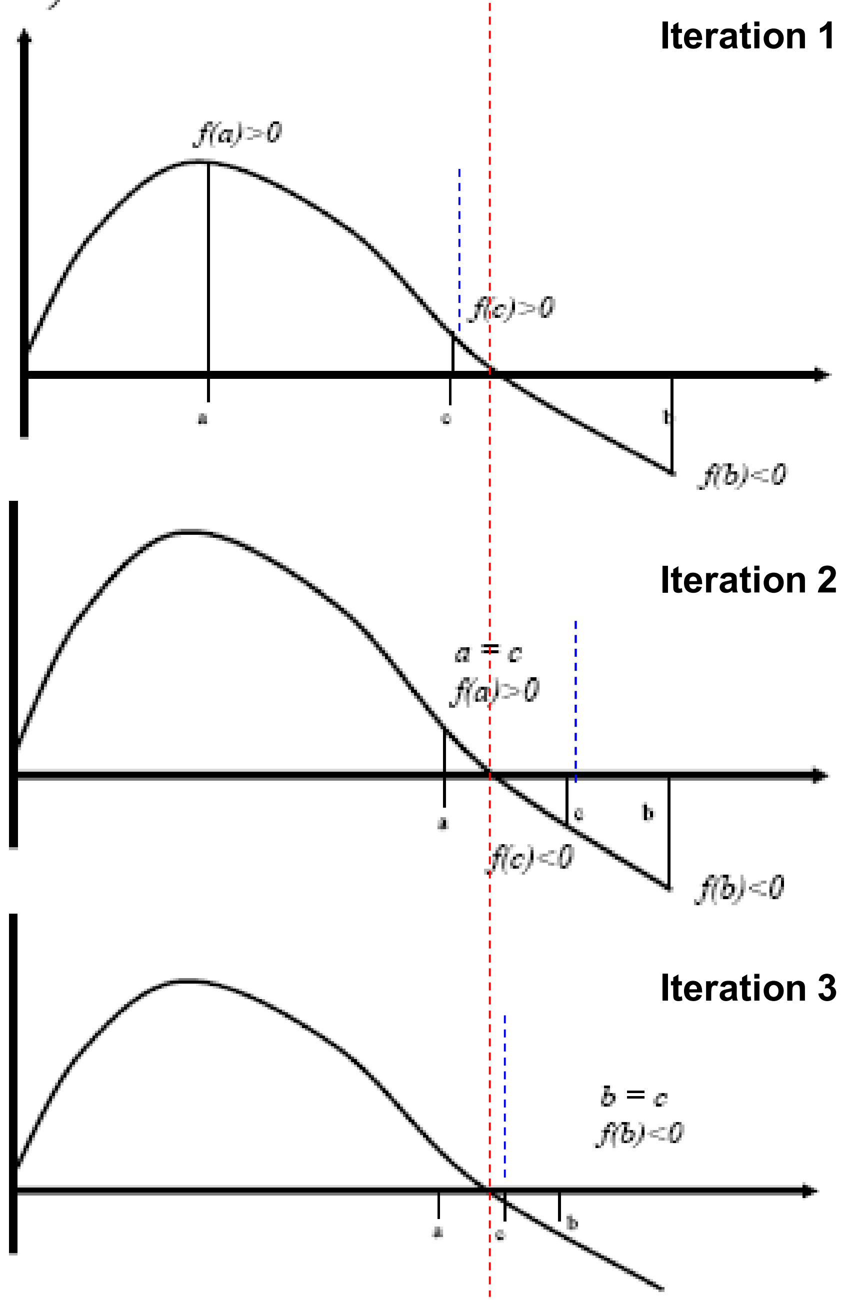
- $c=(a+b)/2$

If $f(a)*f(b)<0$, there is at least one real root between *a* and *b*. The root is within two brackets defined by *a* and *b*.

Numerical estimation
$c=(a+b)/2$

slowly converges to the root

The search interval *b-a* is reduced by ½, and the process can start again until the interval is so small that *f(c)* must be less than the tolerance ε.



Implementation (in computer)

Step 1: Choose lower *a* and upper *b* guesses for the root such that the function *f(x)* changes sign over the interval, i.e., $f(a)f(b)<0$.

Step 2: An estimate of the root *c* where $c=(a+b)/2$.

Step 3: Determine which interval the root lies by:

(i) if $f(a)f(c)<0$, the root lies in the lower interval, set $b=c$.

(ii) if $f(a)f(c)>0$, the root lies in the upper interval, set $a=c$.

(iii) if $f(a)f(c)=0$, the root equal to c, terminate the computation.

Note that step 3(iii) can not be implemented in computer

Example: Finding the root of f(x) between (0, 1)

$$f(x) = 5x^3 - 5x^2 + 6x - 2 = 0$$

iteration	***a***	***b***	***c (root)***	***f*(*a*)**	***f*(c)**	***f*(a)×*f*(c)**	ε_a
1	0	1	0.5	-2	0.375	-0.75	
2	0	0.5	0.25	-2	-0.73438	1.46875	100.00%
3	0.25	0.5	0.375	-0.73438	-0.18945	0.13913	33.33%
4	0.375	0.5	0.4375	-0.18945	0.08667	-0.01642	14.29%
5	0.375	0.4375	0.40625	-0.18945	-0.05246	0.009939	7.69%

Error Definitions

True Value = Approximation + Error

E_t = True value – Approximation (c we choose)

True error

$$\text{True fractional relative error} = \frac{\text{true error}}{\text{true value}}$$

$$\text{True percent relative error, } \varepsilon_t = \frac{\text{true error}}{\text{true value}} \times 100\%$$

- For numerical methods, the true value will be known only when we deal with functions that can be solved analytically (simple systems). In real world applications, we usually not know the answer a priori. Then

$$\varepsilon_{\mathrm{a}} = \left| \frac{\text{Approximate error}}{\text{Approximation}} \right| \times 100\%$$

- *Iterative approach,*

$$\varepsilon_{\mathrm{a}} = \left| \frac{\text{Current approximation - Previous approximation}}{\text{Current approximation}} \right| \times 100\%$$

- Use absolute value.
- Computations are repeated until stopping criterion is satisfied.

$$\varepsilon_a \langle \varepsilon_s$$

Pre-specified % tolerance based on the knowledge of your solution

Termination criteria

At the beginning of computation, the initial guess for the root is *a*

$$x_1^{old} = a, \qquad x_1^{new} = c = \frac{a+b}{2}, \qquad\qquad x_1^{new} - x_1^{old} = \frac{b-a}{2}$$

At the r-th iteration, *a* and *b* are changed. The above relations still apply

Define the approximate percentage relative error

at the r - th iteration

$$\varepsilon_a = \left| \frac{x_r^{new} - x_r^{old}}{x_r^{new}} \right| \times 100\%$$

ε_a tends to zero when iteration ***r*** increases and can be used as termination criteria. For example, if $\varepsilon_a < \varepsilon_s$, the tolerance of error, stop the computation. Otherwise repeat the process.

Advantages of Bisection Method

- The solution is always convergent
- The error is convergent too: The root bracket gets halved with each iteration - guaranteed.

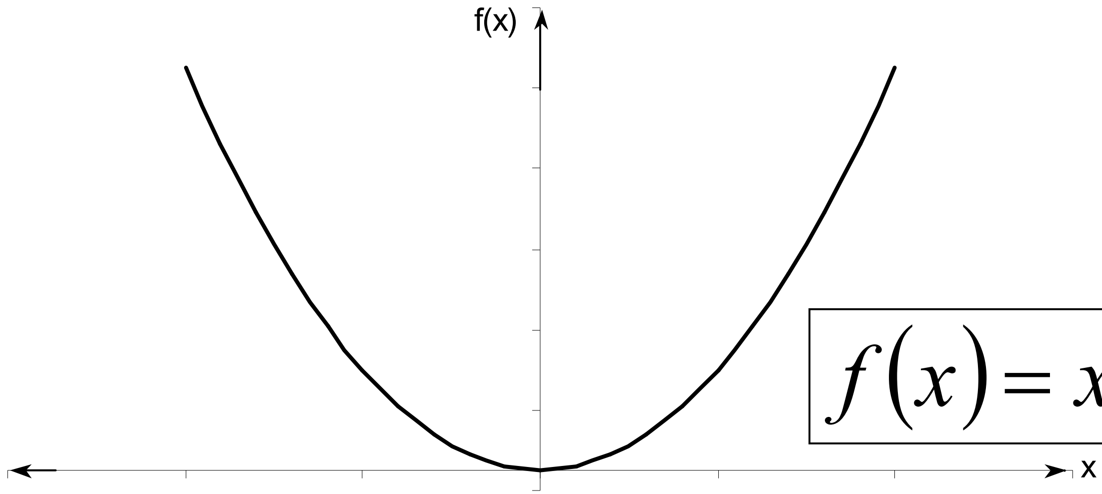
Drawbacks of Bisection Method

- Slow convergence

If one of the initial guesses is close to the root, the convergence is slower.

Drawbacks (continued)

- 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.

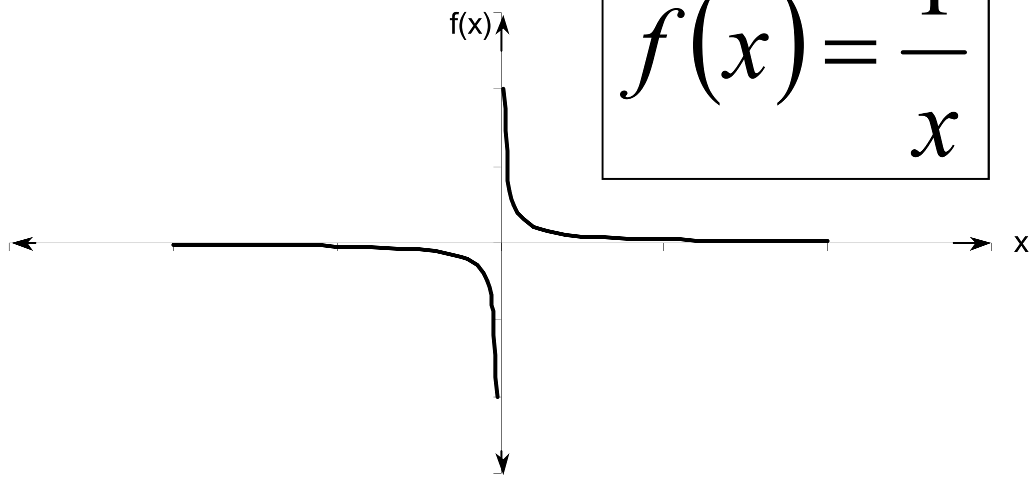


$$\boxed{f(x) = x^4}$$

Drawbacks (continued)

- Function changes sign but root does not exist

$$f(x) = \frac{1}{x}$$



1.2 Open method (Newton-Raphson method)

- Open methods are based on formulas that require only a single starting value of x or two starting values that do not necessarily bracket the root.

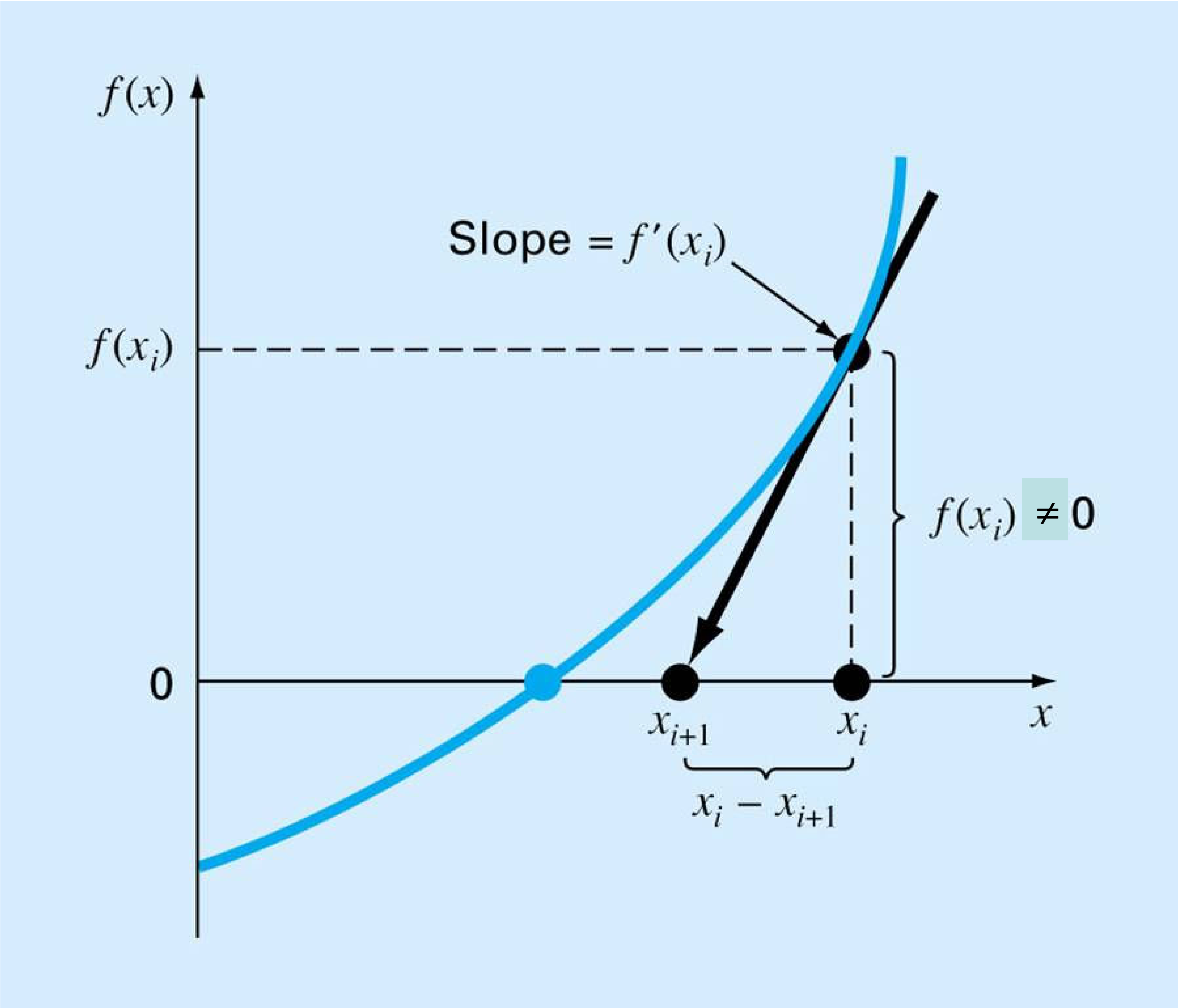
Newton-Raphson method is based on the Taylor expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \cdots + R$$

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

Hence

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$


$f(x)$
Slope = $f'(x_i)$
$f(x_i)$
$f(x_i) \neq 0$
0
x_{i+1}
x_i
x
$x_i - x_{i+1}$

Example /tutorial question

Example 6.3 of textbook [1] (Chapra & Canale) or example in Lecture Notes

$$f(x) = e^{-x} - x$$

The first derivative is $f'(x) = -e^{-x} - 1$; The guess is 0.

$$Hence \qquad x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

Iteration	x_i	ε_t (%)
0	0	
1	0.5	100
2	0.5663110	11.8
3	0.5671431	0.147
4	0.5671433	0.00002

Advantage:

--A convenient method for functions whose derivatives can be evaluated analytically.

--It converges on the true root rapidly.

Drawbacks:

--It may not be convenient for functions whose derivatives cannot be evaluated analytically.

-- It may sometime "diverge", depending on the stating point (initial guess) and how the function behaves. It is caused by, for examples:

(a) Presence of inflection point near the root

(b) Oscillation around a local Min. or Max.

(c) &(d) $f'(x_i) \rightarrow 0$ or near zero.