

~ **Roots of Equations** ~

# Open Methods

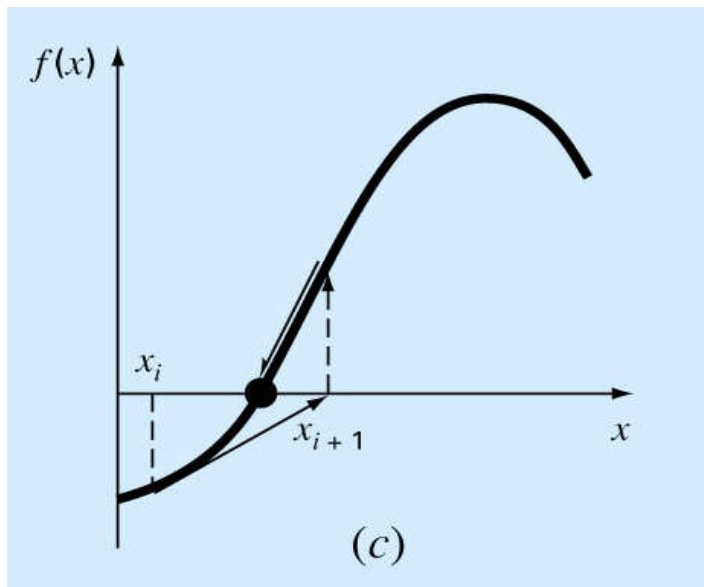
## Chapter 6

Credit: Prof. Lale Yurttas, Chemical Eng., Texas A&M University

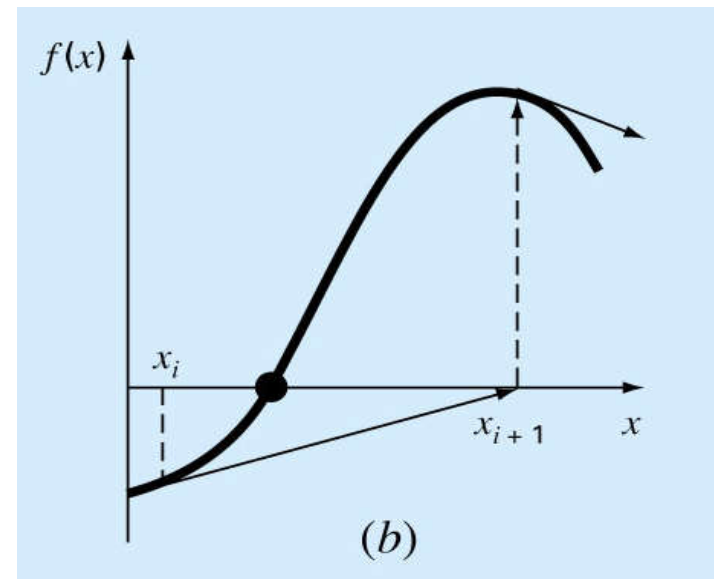
## Open Methods

- Generally use a **single starting value** or two starting values that do not need to bracket the root.

**Open Method** (convergent)



(divergent)



# Simple Fixed-point Iteration

- Rearrange the function so that  $x$  is on the left-hand side of the equation:

$$f(x) = 0 \Rightarrow g(x) = x$$

$$x_k = g(x_{k-1}) \quad x_o \text{ is given, } k = 1, 2, \dots$$

- Bracketing methods are “convergent” if you have a bracket to start with
- Fixed-point methods may sometimes “converge”, depending on the starting point (initial guess) and how the function behaves.

## EXAMPLE:

$$f(x) = x^2 - x - 2 = 0$$

Rewrite it as :  $x = g(x)$

$$x = x^2 - 2$$

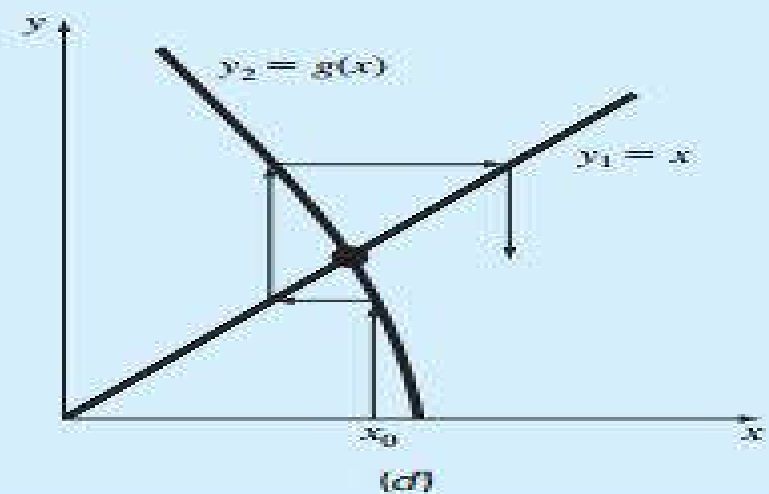
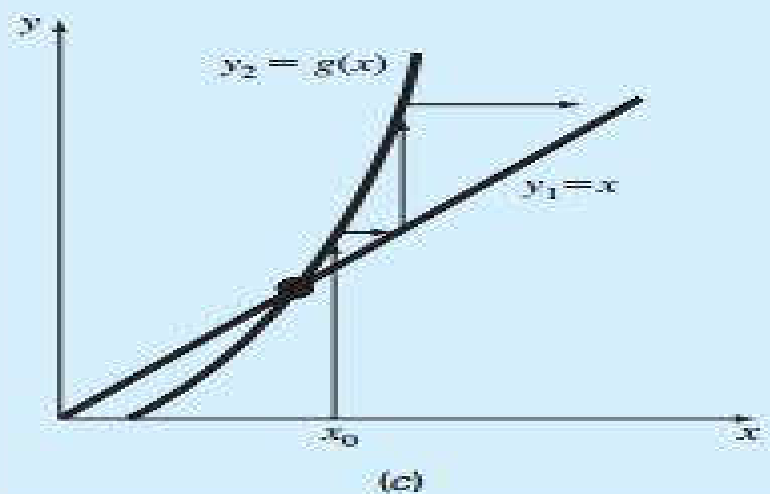
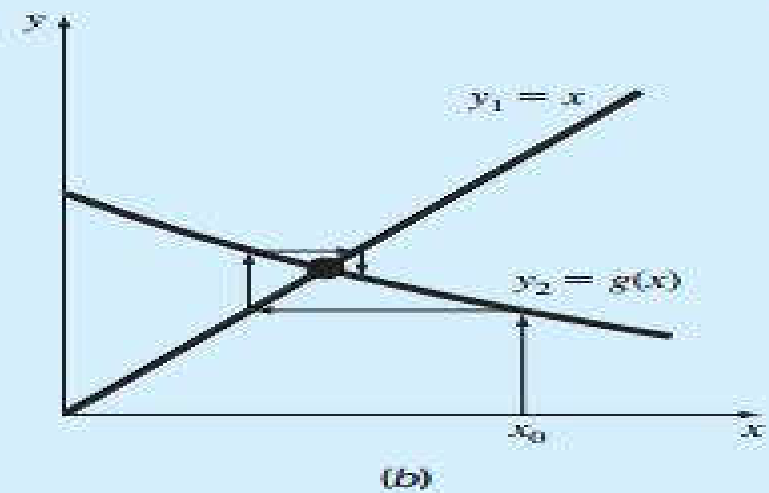
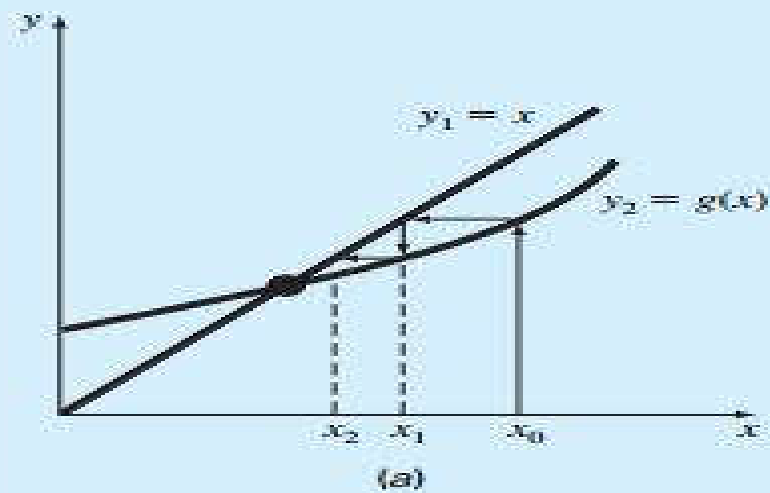
*or*

$$x = \sqrt{x + 2}$$

*or*

$$x = 1 + \frac{2}{x}$$

$\vdots$



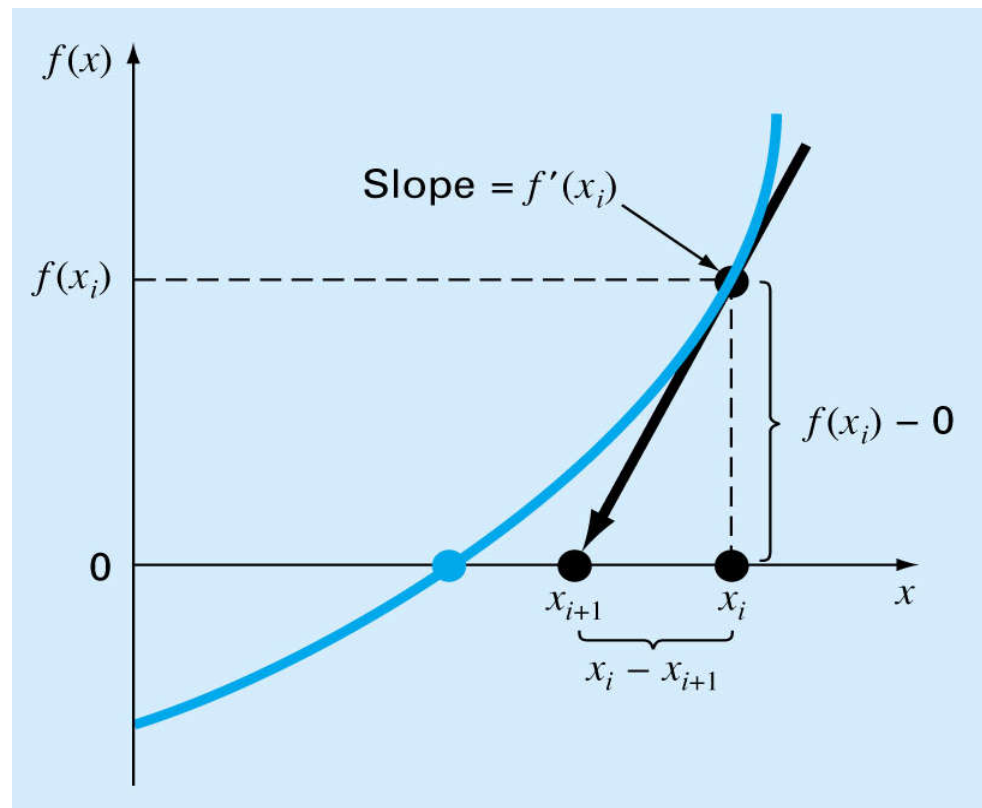
# Newton-Raphson Method

- Most widely used formula for locating roots.
- Can be derived using **Taylor series** or the geometric interpretation of the slope in the figure

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

rearrange to obtain :

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



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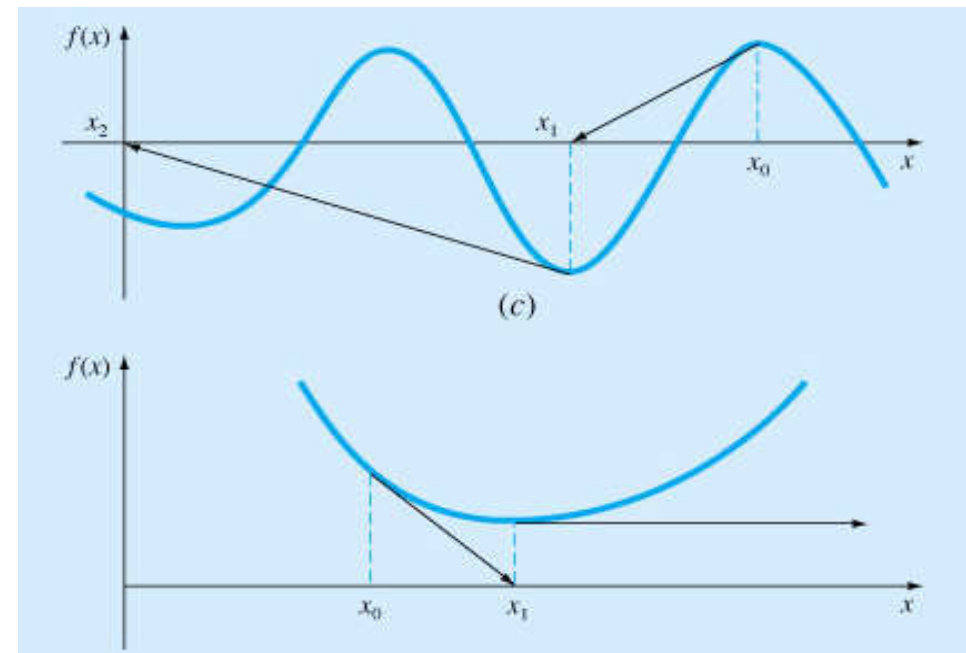
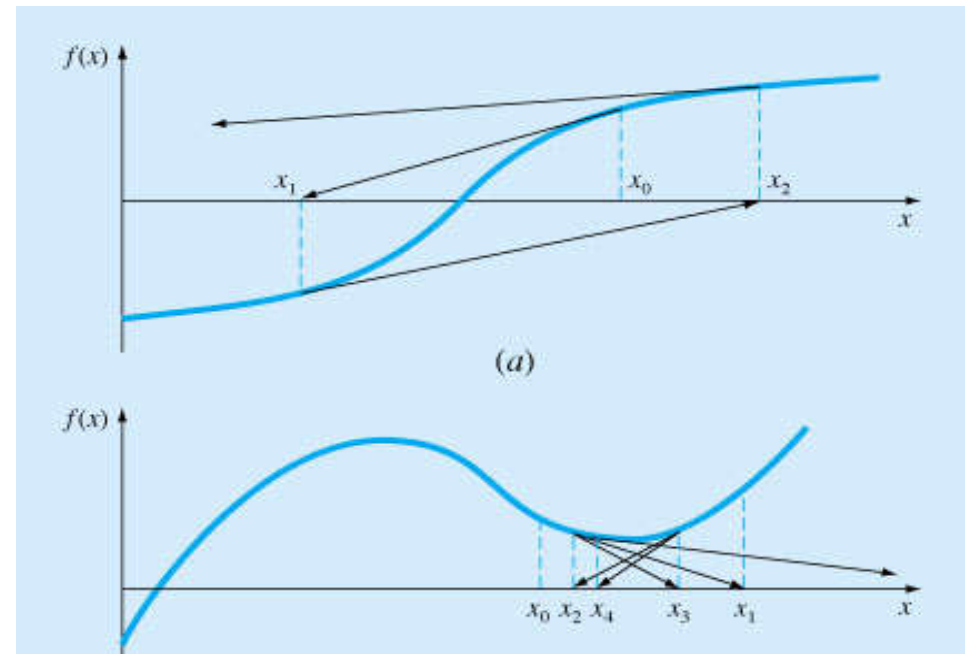
- **Newton-Raphson** is a convenient method if  $f'(x)$  (the derivative) can be evaluated *analytically*
- Rate of convergence is quadratic, i.e. the error is roughly proportional to the square of the previous error

$$E_{i+1} = O(E_i^2)$$

(proof is given in the Text)

**But:**

- it does not always converge  $\Rightarrow \Rightarrow \Rightarrow$
- There is **no convergence criterion**
- Sometimes, it may converge very very slowly (see next slide)



## Example : Slow Convergence

Find the positive roots of :

$$f(x) = x^{10} - 1$$

**N - R Formula :**

$$x_{i+1} = x_i - \frac{x_i^{10} - 1}{10x_i^9} \quad \text{use } x_o = 0.5$$

Iteration	x
0	0.5
1	51.65
2	46.485
3	41.8365
4	37.65285
5	33.887565
.	
.	
38	1.083
$\infty$	1.0000000

## The Secant Method

- If derivative  $f'(x)$  can not be computed **analytically** then we need to compute it **numerically** (*backward finite divided difference method*)
- RESULT:      N-R                      ➔ becomes ➔              SECANT METHOD

**Newton - Raphson :**

$$f'(x_i) = \frac{df}{dx} \cong \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

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

**Secant :** 
$$\mathbf{x}_{i+1} = \mathbf{x}_i - f(\mathbf{x}_i) \frac{\mathbf{x}_i - \mathbf{x}_{i-1}}{f(\mathbf{x}_i) - f(\mathbf{x}_{i-1})} \quad i = 1, 2, 3, \dots$$



# The Secant Method

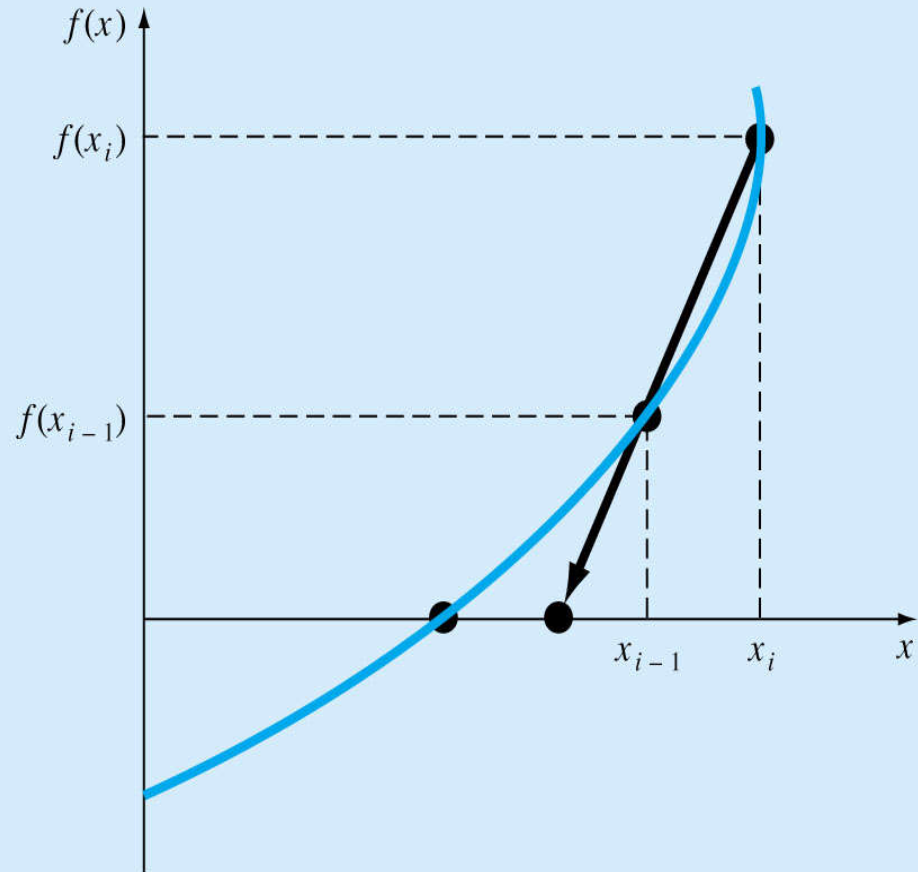
$$x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$$

- Requires two initial estimates  $x_0, x_1$ .

However, it is not a “bracketing” method.

- *The Secant Method* has the same properties as *Newton’s* method.

Convergence is not guaranteed for all  $x_0, f(x)$ .



## Modified Secant Method

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

**Original Secant :** 
$$x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$$

Use a small perturbation fraction  $\delta$  to compute

$$f'(x_i) = \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i} \quad \text{in the original N - R formula :}$$

**Modified Secant:** 
$$x_{i+1} = x_i - f(x_i) \frac{\delta x_i}{f(x_i + \delta x_i) - f(x_i)}$$