

# Roots of Equations (Chapters 5 and 6)

Problem: given  $f(x) = 0$ , find  $x$ .

In general,  $f(x)$  can be any function. For some forms of  $f(x)$ , analytical solutions are available. However, for other functions, we have to design some methods, or algorithms to find either exact, or approximate solution for  $f(x) = 0$ .

We will focus on  $f(x)$

- with single unknown variable,
- not linear, and
- continuous.

Outline:

- Incremental search methods: bisection method, false position method
- Open methods: Newton-Raphson method, Secant method
- Finding repeated roots

### Analytical solutions:

Example 1:  $ax^2 + bx + c = 0$ ,  $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

Example 2:  $ae^x - bx = 0$ . No analytical solution.

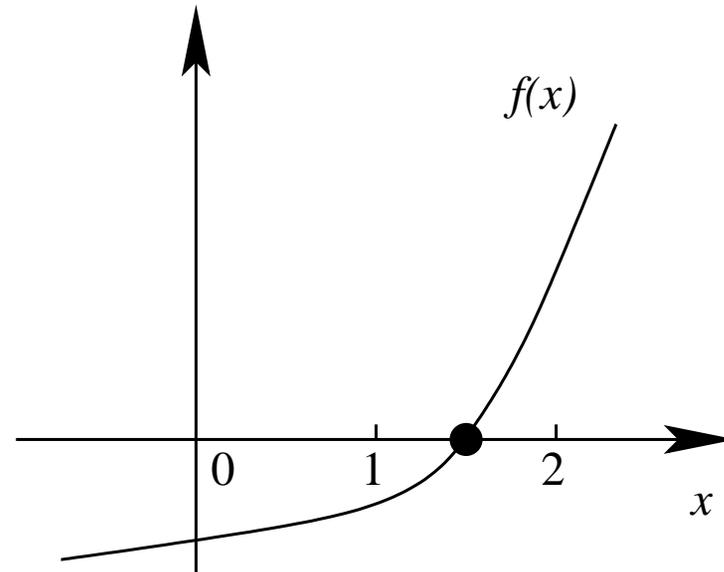
### Straightforward approach: Graphical techniques.

The most straightforward method is to draw a picture of the function and find where the function crosses x-axis.

Graphically find the root: Plot  $f(x)$  for different values of  $x$  and find the intersection with the  $x$  axis.

Graphical methods can be utilized to provide estimates of roots, which can be used as starting guesses for other methods.

Drawbacks: not precise. Different people may have different guesses.



A better method is called incremental search method, which is a general method that most computer-based methods are based on.

## 1 Incremental search methods:

Key idea: The function  $f(x)$  may change signs around the roots.

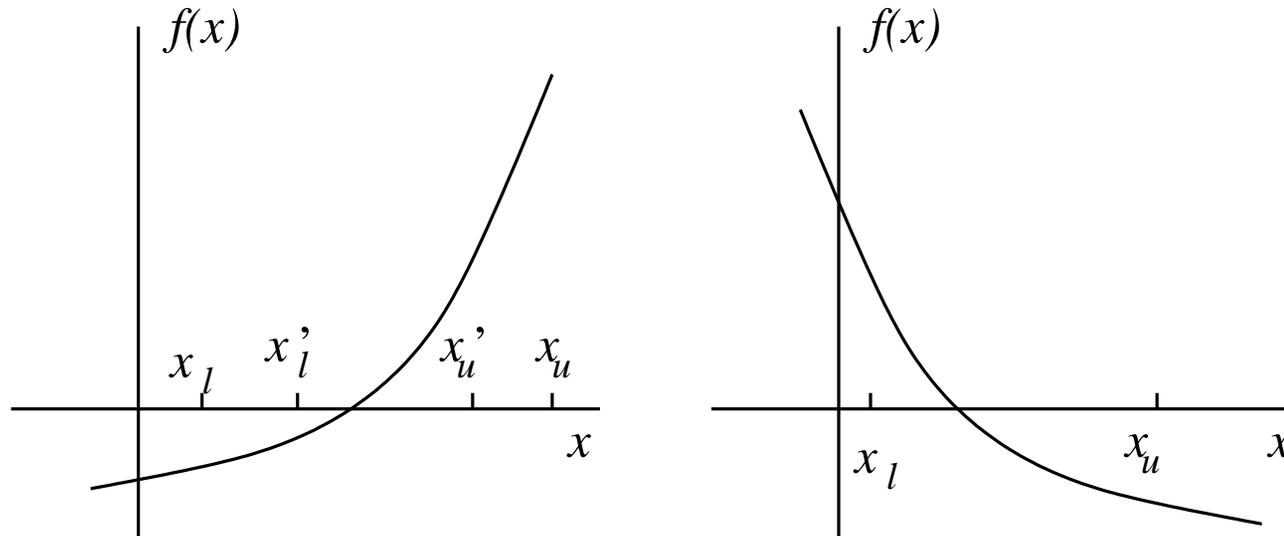


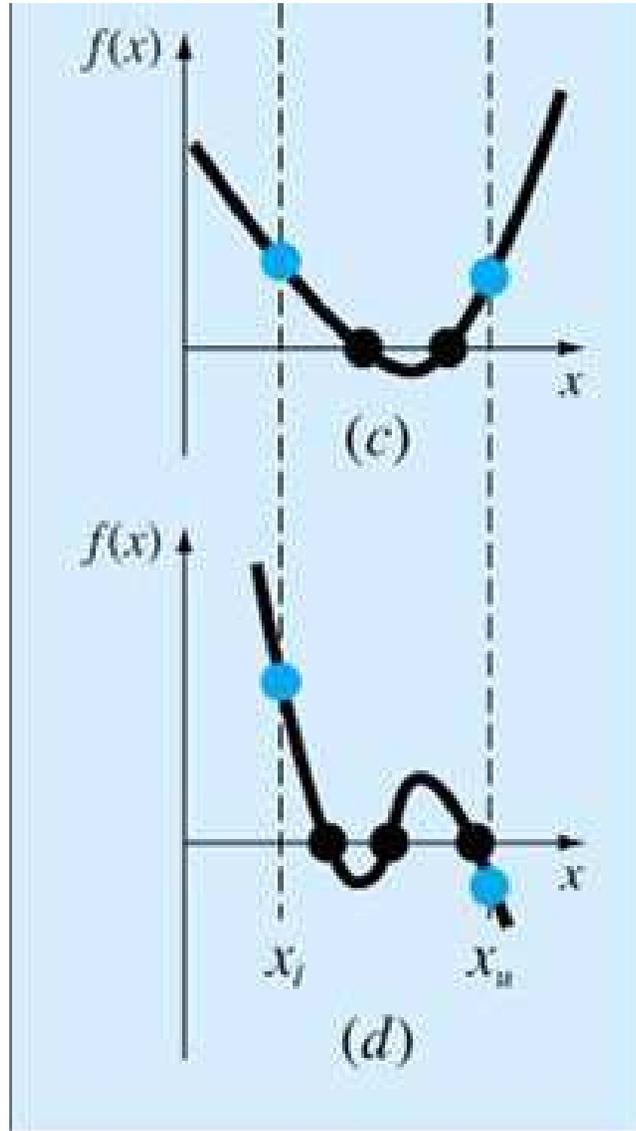
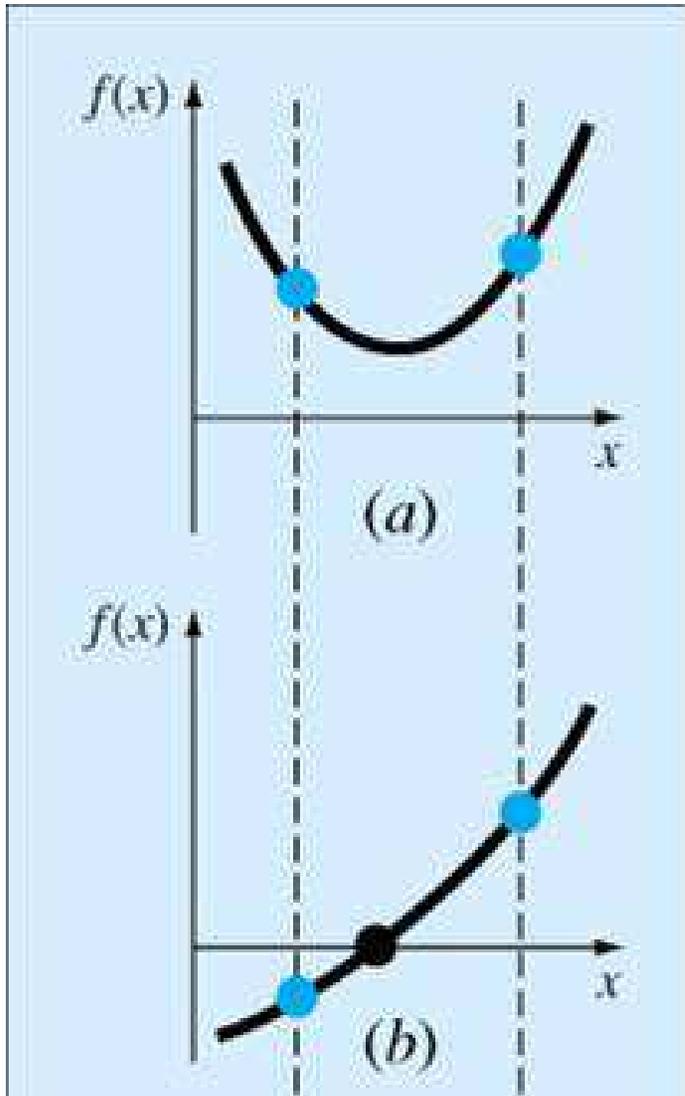
Figure 1: Illustration of incremental search method

Note:  $f(x)$  may not change signs around the roots (see figures on the next page). This case will be dealt with later.

Assume that function  $f(x)$  is real and continuous in interval  $(x_l, x_u)$  and  $f(x)$  has opposite signs at  $x_l$  and  $x_u$ , i.e.,

$$f(x_l) \cdot f(x_u) < 0$$

Then, there is at least one root between  $x_l$  and  $x_u$ .



Next, we can locate the root in a smaller interval until reasonable accuracy is achieved or the root is found.

Based on this, the basic steps in incremental search methods are as follows:

- (1). Locate an interval where the function change signs.
- (2). Divide the interval into a number of sub-intervals.
- (3). Search the sub-interval to accurately locate the sign change.
- (4). Repeat until the root (the location of the sign change) is found.

### **Errors in an iterative approach**

Since getting the exact value of the root is almost impossible during iterations, a termination criterion is needed. (When the error is below a certain stopping threshold, terminate the iterations.)

Define *approximate percentage relative error* as

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

where  $x_r^{\text{new}}$  is the estimated root for the present iteration, and  $x_r^{\text{old}}$  is the estimated root from the previous iteration.

Define *true percentage relative error* as

$$\epsilon_t = \left| \frac{x_t - x_r}{x_t} \right| \times 100\%$$

where  $x_t$  is the true solution of  $f(x) = 0$ , i.e.,  $f(x_t) = 0$ .

In general,  $\epsilon_t < \epsilon_a$ . That is, if  $\epsilon_a$  is below the stopping threshold, then  $\epsilon_t$  is definitely below it as well.

## 2 Bisection (or interval halving) method

Bisection method is an incremental search method where sub-interval for the next iteration is selected by dividing the current interval in half.

### 2.1 Bisection steps

(1). Select  $x_l$  and  $x_u$  such that the function changes signs, i.e.,

$$f(x_l) \cdot f(x_u) < 0$$

(2). Estimate the root as  $x_r$  given by

$$x_r = \frac{x_l + x_u}{2}$$

(3). Determine the next interval:

- If  $f(x_l) \cdot f(x_r) < 0$ , then the root lies in  $(x_l, x_r)$ , set  $x_u = x_r$  and return to Step (2).
- If  $f(x_u) \cdot f(x_r) < 0$ , then the root lies in  $(x_r, x_u)$ , set  $x_l = x_r$  and return to Step (2).

– If  $f(x_u) \cdot f(x_r) = 0$ , then the root has been found. Set the solution  $x = x_r$  and terminate the computation.

(4). If  $\epsilon_a < \epsilon_{threshold}$ ,  $x = x_r$ ; else, repeat the above process.

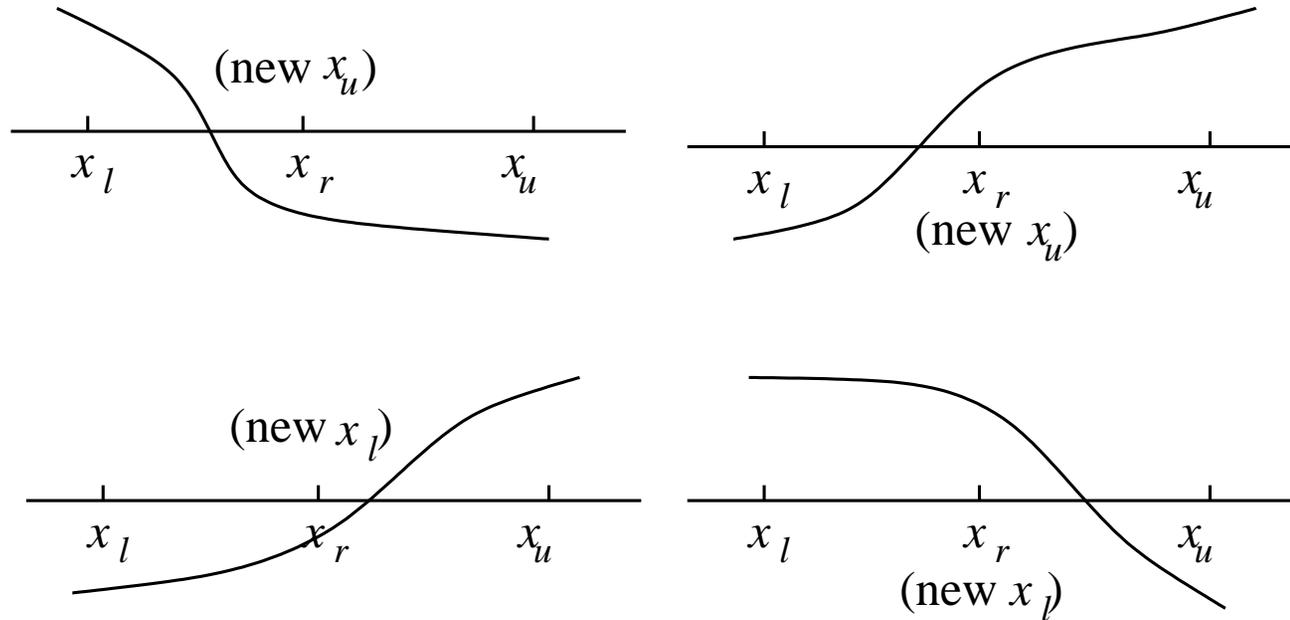


Figure 2: Bisection method

If  $\epsilon_a$  is below a certain threshold (e.g., 1%), stop the iteration. This is, the computation is stopped when the solution does not change much from one iteration to another.

**Example:** Find the root of  $f(x) = e^x - 3 \times x = 0$ .

**Solution:**

1.  $x_l = 0, x_u = 1, f(0) = 1 > 0, f(1) = -0.2817 < 0, x_r = (x_l + x_u)/2 = 0.5, \epsilon = 100\%$ .
2.  $f(0.5) = 0.1487 > 0, x_l = x_r = 0.5, x_u = 1, x_r = (x_l + x_u)/2 = 0.75, \epsilon_a = 33.33\%$ .
3.  $f(0.75) = -0.1330 < 0, x_l = 0.5, x_u = x_r = 0.75, x_r = 0.625, \epsilon_a = 20\%$ .
4.  $f(0.625) = -0.0068 < 0, x_l = 0.5, x_u = x_r = 0.625, x_r = 0.5625, \epsilon_a = 11\%$ .
5.  $f(0.5625) = 0.0676 > 0, x_l = x_r = 0.5625, x_u = x_u = 0.625, x_r = 0.5938, \epsilon_a = 5.3\%$ .
6.  $f(0.5938) = 0.0295 > 0, x_l = x_r = 0.5938, x_u = x_u = 0.625, x_r = 0.6094, \epsilon_a = 2.6\%$ .
7. ...

$x_r: 0.5 \rightarrow 0.75 \rightarrow 0.625 \rightarrow 0.5625 \rightarrow 0.5938 \rightarrow 0.6094 \rightarrow 0.6172 \rightarrow 0.6211 \rightarrow 0.6191 \rightarrow 0.6182 \rightarrow 0.6187 \rightarrow 0.6189 \rightarrow 0.6190 \rightarrow 0.6191$

### Bisection Method (between 0 and 1)

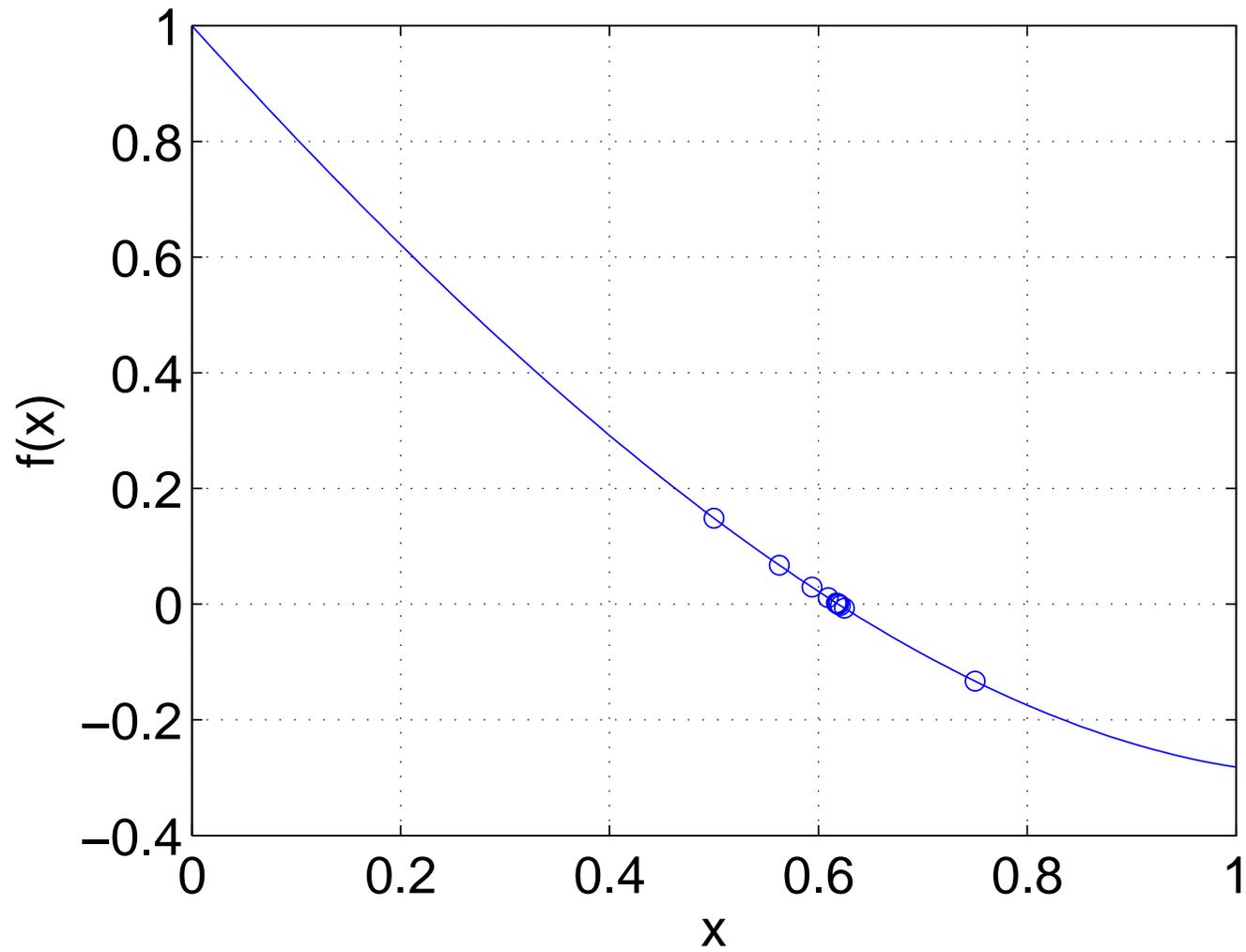


Figure 3: Example of using Bisection method,  $f(x) = e^x - 3 \times x = 0$

## 2.2 Evaluation of $\epsilon_a$

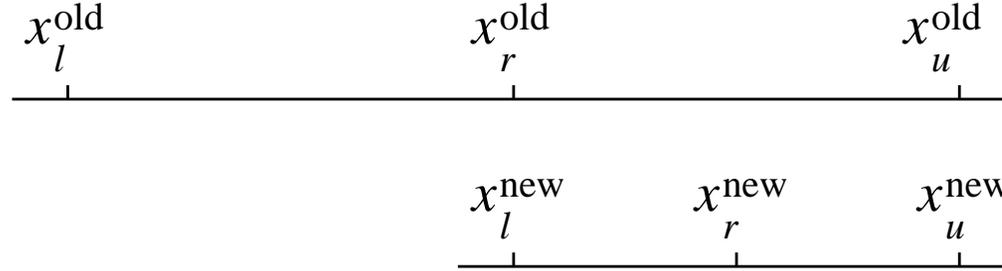


Figure 4: Evaluation of  $\epsilon_a$

$$\epsilon_a = \left| \frac{x_r^{\text{new}} - x_r^{\text{old}}}{x_r^{\text{new}}} \right|$$

$$x_r^{\text{new}} = \frac{1}{2}(x_l^{\text{new}} + x_u^{\text{new}})$$

$$x_r^{\text{old}} = x_l^{\text{new}}$$

Therefore,

$$x_r^{\text{new}} - x_r^{\text{old}} = \frac{1}{2}x_l^{\text{new}} + \frac{1}{2}x_u^{\text{new}} - x_l^{\text{new}} = \frac{1}{2}(x_u^{\text{new}} - x_l^{\text{new}})$$

and

$$\epsilon_a = \left| \frac{\frac{1}{2}(x_u^{\text{new}} - x_l^{\text{new}})}{\frac{1}{2}(x_u^{\text{new}} + x_l^{\text{new}})} \right| \times 100\%$$

or

$$\epsilon_a = \frac{x_u - x_l}{x_u + x_l} \times 100\%$$

That is, the relative error can be found before starting the iteration.

### 2.3 Finding the number of iterations

Initially (iteration 0), the absolute error is

$$E_a^0 = x_u^0 - x_l^0 = \Delta_x^0$$

where superscript indicates the iteration number.

After first iteration, the absolute error is halved. That is

$$E_a^1 = \frac{1}{2}E_a^0 = \frac{\Delta_x^0}{2}$$

After  $n$  iterations,

$$E_a^n = \frac{1}{2}E_a^{n-1} = \frac{\Delta_x^0}{2^n}$$

If the desired absolute error is  $E_{a,d}$ , then

$$E_a^n \leq E_{a,d}$$

which is equivalent to

$$\frac{\Delta_x^0}{2^n} \leq E_{a,d} \Rightarrow n \geq \log_2 \frac{\Delta_x^0}{E_{a,d}}$$

The minimum  $n$  is

$$\left\lceil \log_2 \frac{\Delta_x^0}{E_{a,d}} \right\rceil = \left\lceil \frac{\log_{10} \frac{\Delta_x^0}{E_{a,d}}}{\log_{10} 2} \right\rceil$$

**Example:**

Find the roots of function  $f(x) = x^3 - 2x^2 + 0.25x + 0.75$ .

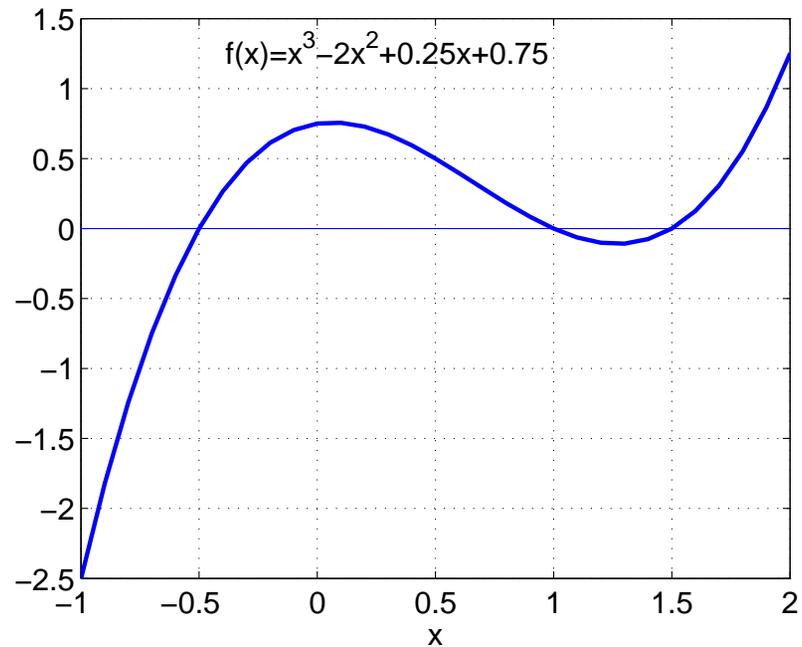
Solution:

To find the exact roots of  $f(x)$ , we first factorize  $f(x)$  as

$$\begin{aligned} f(x) &= x^3 - 2x^2 + 0.25x + 0.75 \\ &= (x - 1)(x^2 - x - 0.75) \\ &= (x - 1) \cdot (x - 1.5) \cdot (x + 0.5) \end{aligned}$$

Thus,  $x = 1$ ,  $x = 1.5$  and  $x = -0.5$  are the exact roots of  $f(x)$ .

- $x_l = -1$ ,  $x_u = 2$ , the result converges to  $x_r = -0.5$ .
- $x_l = -2$ ,  $x_u = 2$ , the result converges to  $x_r = -0.5$ .
- $x_l = -1$ ,  $x_u = 8$ , the result converges to  $x_r = 1.5$ .



### 3 Newton-Raphson method

#### 3.1 Iterations

The Newton-Raphson method uses the slope (tangent) of the function  $f(x)$  at the current iterative solution  $(x_i)$  to find the solution  $(x_{i+1})$  in the next iteration.

The slope at  $(x_i, f(x_i))$  is given by

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

Then  $x_{i+1}$  can be solved as

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

which is known as the Newton-Raphson formula.

Relative error:  $\epsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$ .

Iterations stop if  $\epsilon_a \leq \epsilon_{threshold}$ .

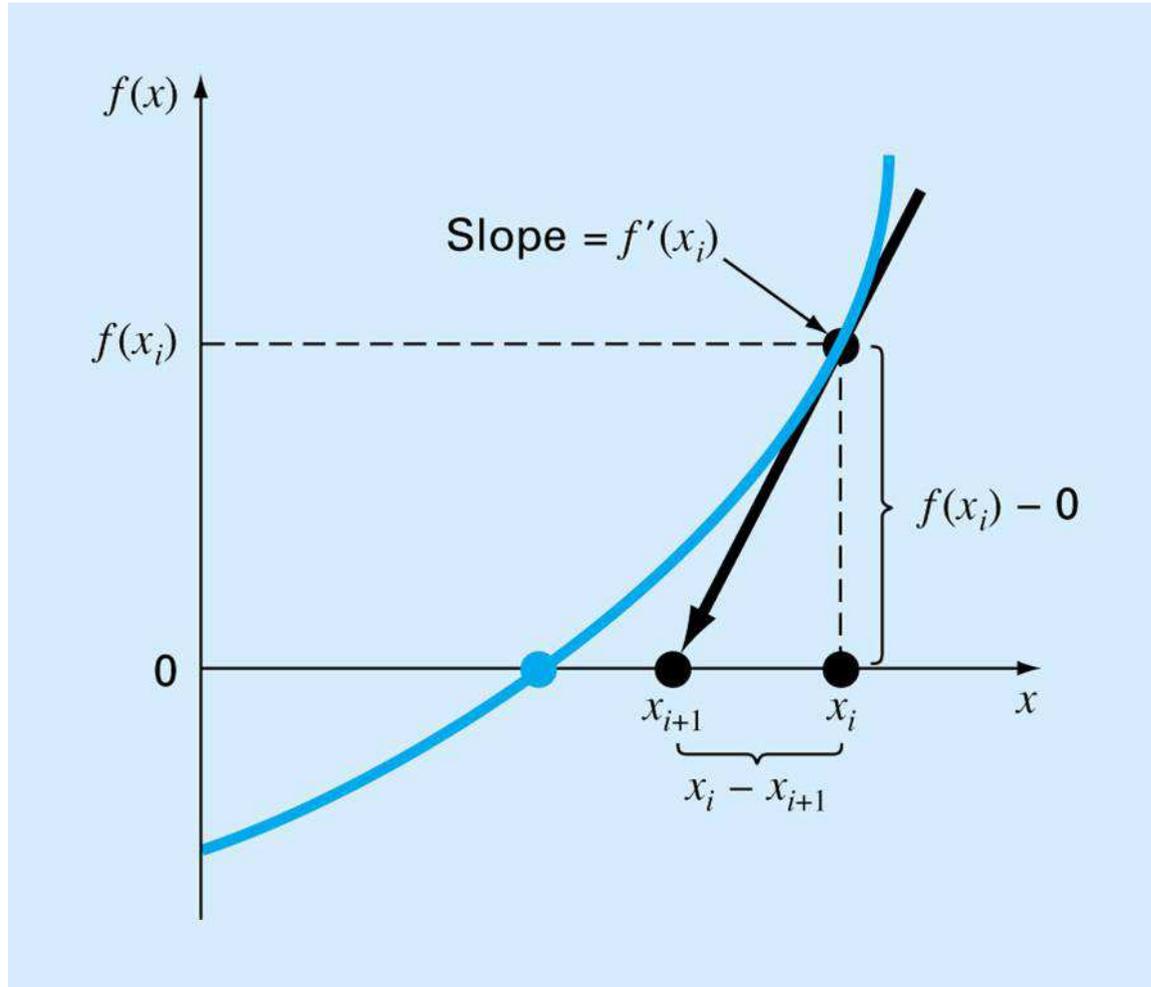


Figure 5: Newton-Raphson method to find the roots of an equation

Example: Find the root of  $e^{-x} - 3x = 0$ .

Solution:

$$f(x) = e^{-x} - 3x$$

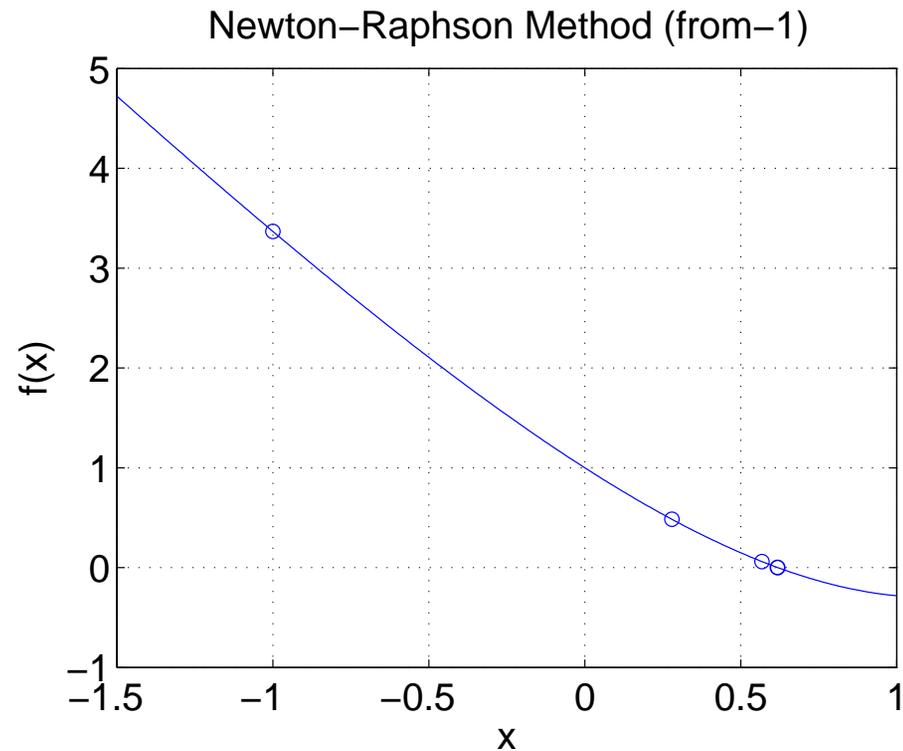
$$f'(x) = -e^{-x} - 3$$

With these, the Newton-Raphson solution can be updated as

$$x_{i+1} = x_i - \frac{e^{-x_i} - 3x_i}{-e^{-x_i} - 3}$$

$-1 \rightarrow 0.2795 \rightarrow 0.5680 \rightarrow 0.6172 \rightarrow 0.6191 \rightarrow 0.6191$

Converges much faster than the bisection method.



### 3.2 Errors and termination condition

The approximate percentage relative error is

$$\epsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\%$$

The Newton-Raphson iteration can be terminated when  $\epsilon_a$  is less than a certain threshold (e.g., 1%).

### 3.3 Error analysis of Newton-Raphson method using Taylor series

Let  $x_t$  be the true solution to  $f(x) = 0$ . That is

$$f(x_t) = 0$$

According to the Taylor's theorem, we have

$$f(x_t) = f(x_i) + f'(x_i)(x_t - x_i) + \frac{f''(\alpha)}{2}(x_t - x_i)^2$$

where  $\alpha$  is an unknown value between  $x_t$  and  $x_i$ . Since  $f(x_t) = 0$ , the above equation becomes

$$f(x_i) + f'(x_i)(x_t - x_i) + \frac{f''(\alpha)}{2}(x_t - x_i)^2 = 0 \quad (1)$$

In Newton-Raphson method, we use the following iteration:

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

That is

$$f(x_i) + f'(x_i)(x_{i+1} - x_i) = 0 \quad (2)$$

Subtracting (2) from (1), we have

$$f'(x_i)(x_t - x_{i+1}) + \frac{f''(\alpha)}{2}(x_t - x_i)^2 = 0$$

Denoting  $e_i = x_t - x_i$ , which is the error in the  $i$ -th iteration, we have

$$f'(x_i)e_{i+1} + \frac{f''(\alpha)}{2}(e_i)^2 = 0$$

With convergence,  $x_i \rightarrow x_t$ , and  $\alpha \rightarrow x_t$ . Then

$$e_{i+1} = -\frac{f''(x_t)}{2f'(x_t)}e_i^2$$

and

$$|e_{i+1}| = \left| \frac{f''(x_t)}{2f'(x_t)} \right| e_i^2$$
$$|e_{i+1}| \propto |e_i|^2$$

The error in the current iteration is proportional to the square of the previous error. That is, we have quadratic convergence with the Newton-Raphson method. The number of correct decimal places in a Newton-Raphson solution doubles after each iteration.

Drawbacks of the Newton-Raphson method: (see Fig. 6.6 in [Chapra])

- It cannot handle repeated roots

- The solution may diverge near a point of inflection.
- The solution may oscillate near local minima or maxima.
- With near-zero slope, the solution may diverge or reach a different root.

**Example:**

Find the roots of function  $f(x) = x^3 - 2x^2 + 0.25x + 0.75$ .

Solution:

To find the exact roots of  $f(x)$ , we first factorize  $f(x)$  as

$$\begin{aligned} f(x) &= x^3 - 2x^2 + 0.25x + 0.75 \\ &= (x - 1)(x^2 - x - 0.75) \\ &= (x - 1) \cdot (x - 1.5) \cdot (x + 0.5) \end{aligned}$$

Thus,  $x = 1$ ,  $x = 1.5$  and  $x = -0.5$  are the exact roots of  $f(x)$ .

To find the roots using the Newton-Raphson methods, write the iteration formula as

$$\begin{aligned} x_{i+1} &= x_i - \frac{f(x_i)}{f'(x_i)} \\ &= x_i - \frac{x^3 - 2x^2 + 0.25x + 0.75}{3x^2 - 4x + 0.25} \end{aligned}$$

- $x_0 = -1, x_1 = -0.6552, x_2 = -0.5221, x_3 = -0.5005, x_4 = -0.5000, x_5 = -0.5000$ .
- $x_0 = 0, x_1 = -3, x_2 = -1.8535, x_3 = -1.1328, x_4 = -0.7211, x_5 = -0.5410, x_6 = -0.5018, x_7 = -0.5000, x_8 = -0.5000$ .

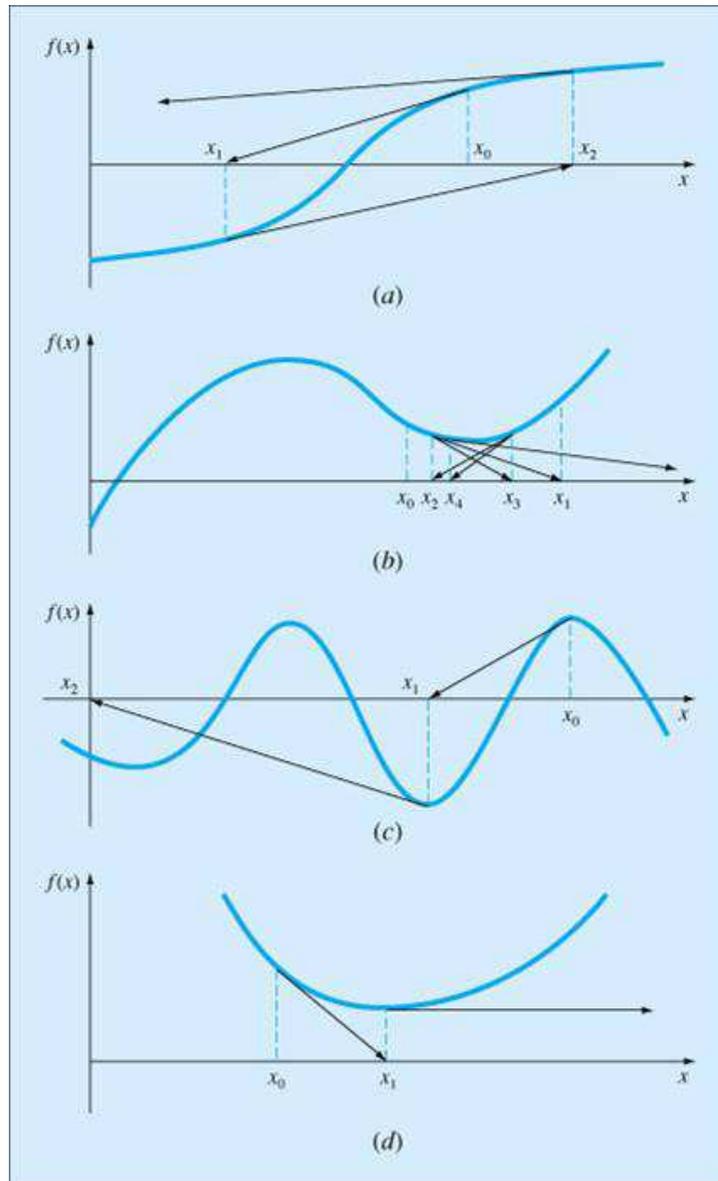


Figure 6: Drawbacks of using NR method

- $x_0 = 0.5, x_1 = 1, x_2 = 1.$
- $x_0 = 1.3, x_1 = 1.5434, x_2 = 1.5040, x_3 = 1.5000, x_4 = 1.5000.$
- $x_0 = 1.25, x_1 = -0.5000, x_2 = -0.5000.$

## 4 Secant method

In order to implement the Newton-Raphson method,  $f'(x)$  needs to be found analytically and evaluated numerically. In some cases, the analytical (or its numerical) evaluation may not be feasible or desirable.

The Secant method is to evaluate the derivative online using two-point differencing.

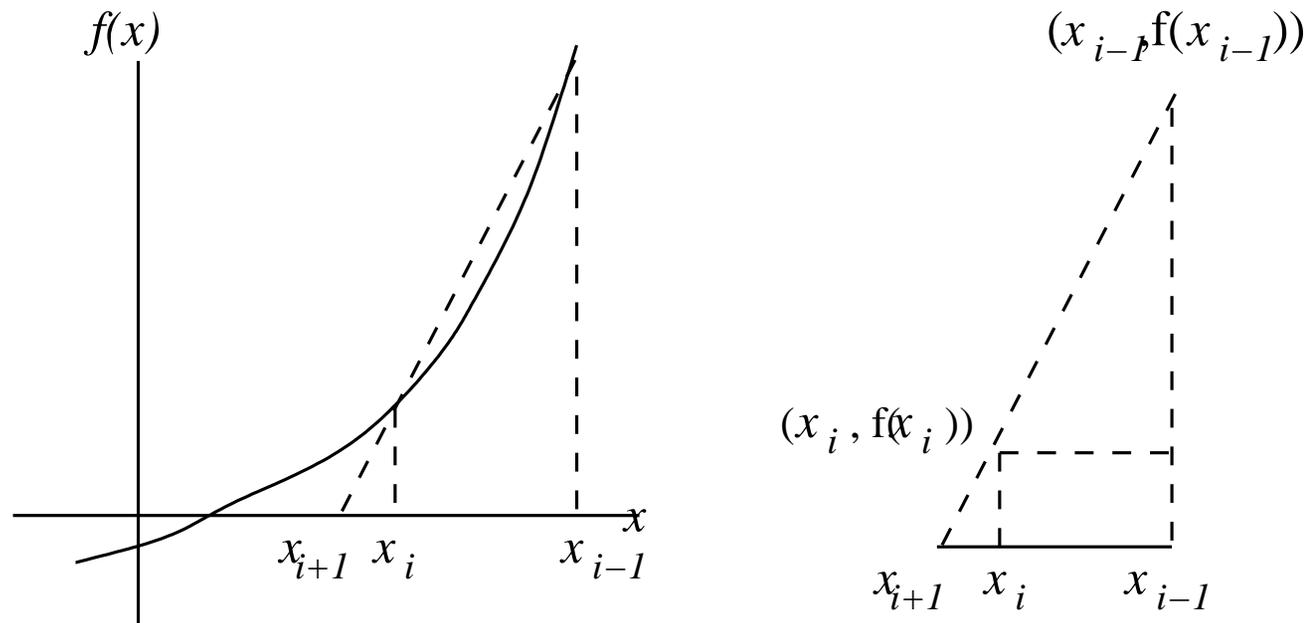


Figure 7: Secant method to find the roots of an equation

As shown in the figure,

$$f'(x) \approx \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

Then the Newton-Raphson iteration can be modified as

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

which is the Secant iteration.

The performance of the Secant iteration is typically inferior to that of the Newton-Raphson method.

Example:  $f(x) = e^x - 3x = 0$ , find  $x$ .

Solution:

$$x_0 = -1.1, x_1 = -1, x_2 = x_1 - \frac{f(x_1)(x_1 - x_0)}{f(x_1) - f(x_0)} = 0.2709, \epsilon_a = \left| \frac{x_2 - x_1}{x_2} \right| \times 100\% = 469.09\%$$

$$x_1 = -1, x_2 = 0.2709, x_3 = x_2 - \frac{f(x_2)(x_2 - x_1)}{f(x_2) - f(x_1)} = 0.4917, \epsilon_a = \left| \frac{x_3 - x_2}{x_3} \right| \times 100\% = 44.90\%$$

$$x_2 = 0.2709, x_3 = 0.4917, x_4 = x_3 - \frac{f(x_3)(x_3 - x_2)}{f(x_3) - f(x_2)} = 0.5961, \epsilon_a = \left| \frac{x_4 - x_3}{x_4} \right| \times 100\% = 17.51\%$$

$$x_5 = 0.6170, \epsilon_a = 3.4\%$$

$$x_6 = 0.6190, \epsilon_a = 0.32\%$$

$$x_7 = 0.6191, \epsilon_a = 5.93 \times 10^{-5}$$

## 5 False position method

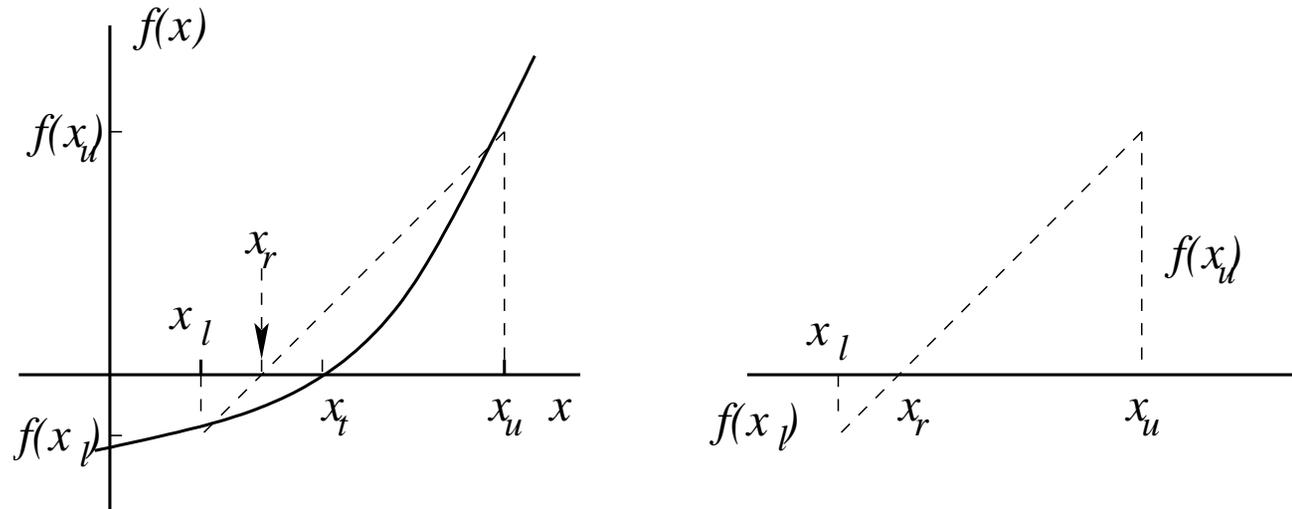


Figure 8: False position method to find the roots of an equation

Idea: if  $f(x_l)$  is closer to zero than  $f(x_u)$ , then the root is more likely to be closer to  $x_l$  than to  $x_u$ . (NOT always true!)

False position steps:

- (1). Find  $x_l, x_u, x_l < x_u, f(x_l)f(x_u) < 0$
- (2). Estimate  $x_r$  using similar triangles:

$$\frac{-f(x_l)}{f(x_u)} = \frac{x_r - x_l}{x_u - x_r}$$

Find  $x_r$  as

$$x_r = \frac{[f(x_l) - f(x_u)]x_u + f(x_u)(x_u - x_l)}{f(x_l) - f(x_u)}$$

or

$$x_r = x_u - \frac{f(x_u)(x_u - x_l)}{f(x_u) - f(x_l)}$$

(3). Determine next iteration interval

- If  $f(x_l) \cdot f(x_r) < 0$ , then the root lies in  $(x_l, x_r)$ , set  $x_u = x_r$  and return to Step (2).
- If  $f(x_u) \cdot f(x_r) < 0$ , then the root lies in  $(x_r, x_u)$ , set  $x_l = x_r$  and return to Step (2).
- If  $f(x_u) \cdot f(x_r) = 0$ , then the root has been found. Set the solution  $x = x_r$  and terminate the computation.

(4). If  $\epsilon_a < \epsilon_{threshold}$ ,  $x = x_r$ ; else, back to (2).

False position method is one of the incremental search methods.

In general, false position method performs better than bisection method. However, special case exists (see fig. 5.14 in textbook).

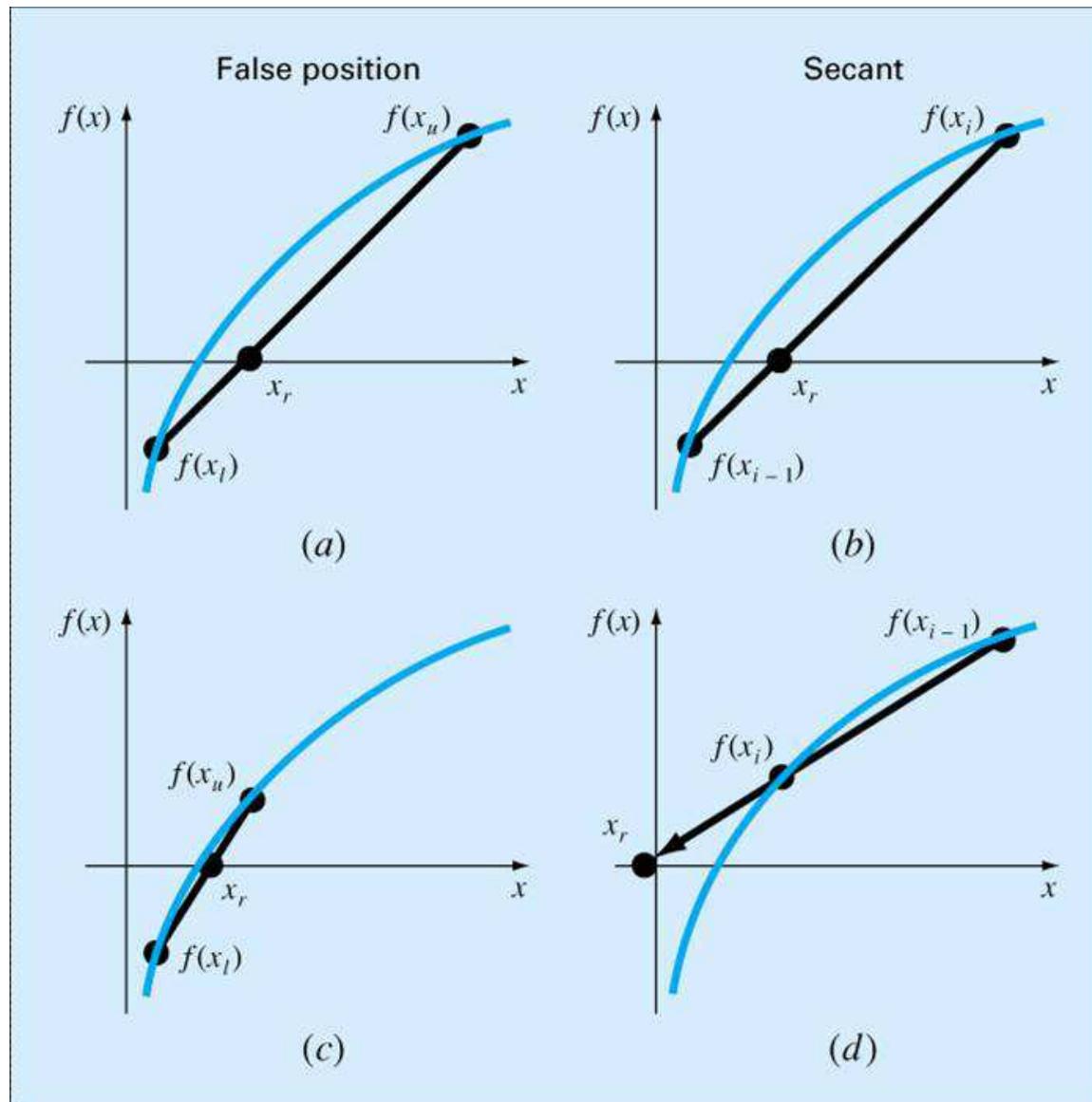
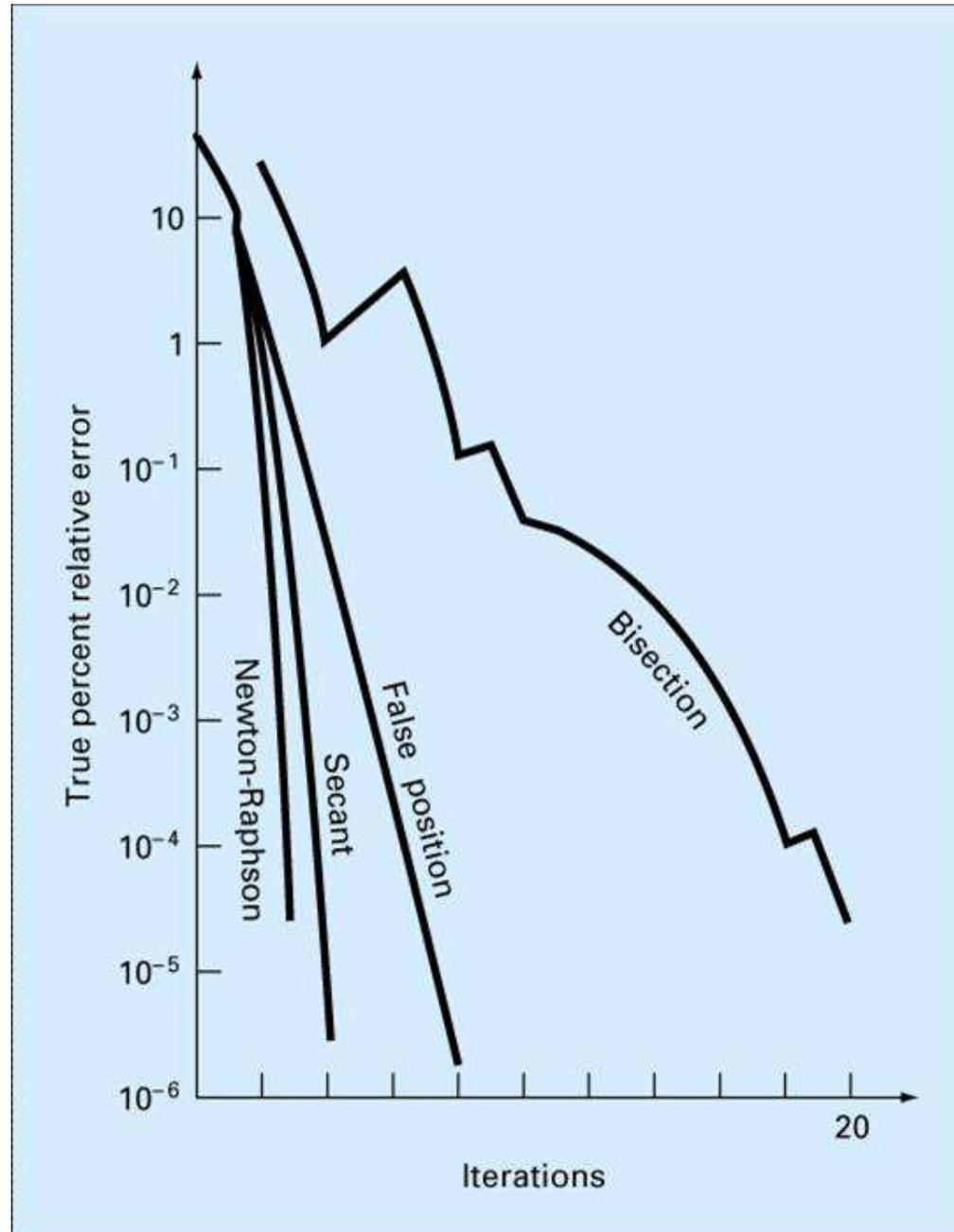


Figure 9: Comparison between false position and Secant methods



## 6 Handling repeated (multiple) roots

Examples of multiple roots:

- $f(x) = x^2 - 4x + 3 = (x - 1)(x - 3)$  has unrepeated roots:  $x = 1, x = 3$
- $f(x) = (x - 1)^2(x - 3)$  has 2 repeated roots at  $x = 1$
- $f(x) = (x - 1)^3(x - 3)$  has 3 repeated roots at  $x = 1$
- $f(x) = (x - 1)^4(x - 3)$  has 4 repeated roots at  $x = 1$

Observations:

- The sign of the function does not change around even multiple roots — bisection and false position methods do not work
- Both  $f(x)$  and  $f'(x)$  go to zero around multiple roots — Newton-Raphson and secant methods may converge slowly or even diverge.

### 6.1 Modified Newton-Raphson method

Fact: Both  $f(x)$  and  $u(x) = \frac{f(x)}{f'(x)}$  have the same roots, but  $u(x)$  has better convergence properties.

Idea: to find the roots of  $u(x)$  instead of  $f(x)$ .

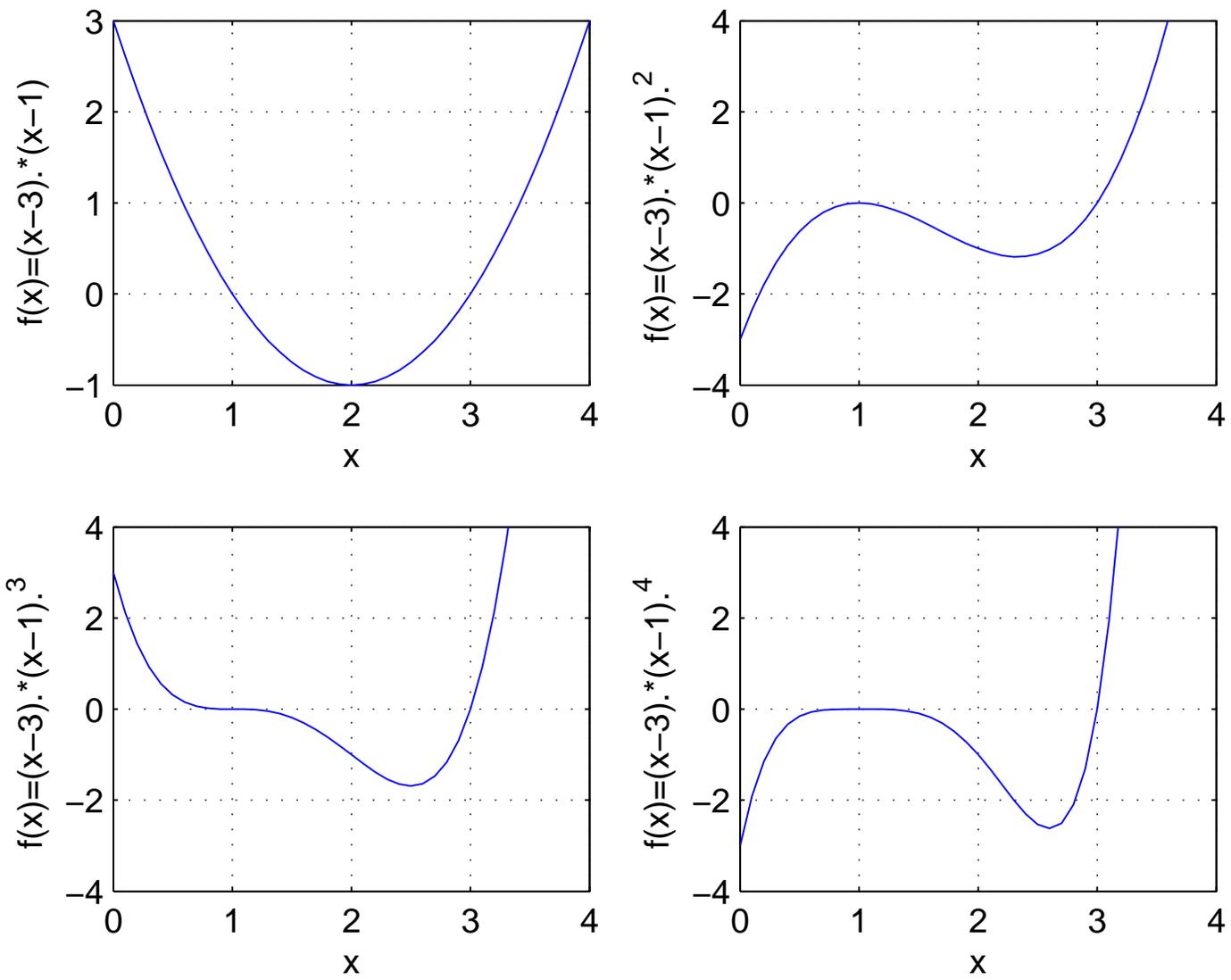


Figure 10: Repeated roots

The Newton-Raphson method iteration for  $u(x)$ :

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

$$u'(x) = \frac{[f'(x)]^2 - f(x)f''(x)}{[f'(x)]^2}$$

$$x_{i+1} = x_i - \frac{[f'(x_i)]^2}{[f'(x_i)]^2 - f(x_i)f''(x_i)} \frac{f(x_i)}{f'(x_i)}$$

or

$$x_{i+1} = x_i - \frac{f(x_i)f'(x_i)}{[f'(x_i)]^2 - f(x_i)f''(x_i)}$$

Modified Newton-Raphson method has quadratic convergence even for multiple roots.

$x_t$  is an unrepeated root of  $u(x) = 0$

$f(x)$  has  $n$  repeated roots,  $n \geq 2$

$$f(x) = g(x) \cdot (x - x_t)^n$$

where  $g(x_t) \neq 0$ . Then

$$\begin{aligned} f'(x) &= g'(x)(x - x_t)^n + g(x)n(x - x_t)^{n-1} \\ &= (x - x_t)^{n-1} [g'(x)(x - x_t) + ng(x)] \end{aligned}$$

and

$$\begin{aligned} u(x) &= \frac{f(x)}{f'(x)} \\ &= \frac{g(x) \cdot (x - x_t)^n}{(x - x_t)^{n-1} [g'(x)(x - x_t) + ng(x)]} \\ &= \frac{g(x) \cdot (x - x_t)}{g'(x)(x - x_t) + ng(x)} \end{aligned}$$

Therefore,  $x_t$  is an unrepeated root of  $u(x) = 0$ .